Stochastic Parameterization: Towards a new view of Weather and Climate Models

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ABSTRACT

The last decade has seen the success of stochastic parameterizations in short-term, medium-range and seasonal ensembles: operational weather centers now routinely use stochastic parameterization schemes to better represent model inadequacy and improve the quantification of forecast uncertainty. Developed initially for numerical weather prediction, the inclusion of stochastic parameterizations not only provides more skillful estimates of uncertainty, but it is also extremely promising for reducing longstanding climate biases and is relevant for determining the climate response to forcings such as e.g., an increase of CO2.

This article highlights recent developments from different research groups which show that the stochastic representation of unresolved processes in the atmosphere, oceans, land surface and cryosphere of comprehensive weather and climate models (a) gives rise to more reliable probabilistic forecasts of weather and climate and (b) reduces systematic model bias.

We make a case that the use of mathematically stringent methods for derivation of stochastic dynamic equations will lead to substantial improvements in our ability to accurately simulate weather and climate at all scales. Recent work in mathematics, statistical mechanics and turbulence is reviewed, its relevance for the climate problem demonstrated, and future research directions outlined.

CAPSULE (20-30 words)

Stochastic parameterizations - empirically derived, or based on rigorous mathematical and statistical concepts - have great potential to increase the predictive capability of next generation weather and climate models.

The need for stochastic parameterizations

Numerical weather and climate modeling is based on the discretization of the continuous equations of motion. Such models can be characterized in terms of their dynamical core, which describes the resolved scales of motion, and the physical parameterizations, which provide estimates of the grid-scale effect of processes, that cannot be resolved. This general approach has been hugely successful in that skillful predictions of weather and climate are now routinely made (e.g. Bauer et al. 2015). However, it has become apparent through the verification of these predictions that current state-of the art models still exhibit persistent and systematic shortcomings due to an inadequate representation of unresolved processes.

Despite the continuing increase of computing power, which allows numerical weather and climate prediction models to be run with ever higher resolution, the multi-scale nature s of geophysical fluids means that many important physical processes (e.g. tropical convection, gravity wave drag, micro-physical processes) are still not resolved.

Moreover, for climate simulations, a decision must be made as to whether computational resources should be used to increase the representation of subgrid physical processes or to build a comprehensive Earth-System Model, by including additional climate components such as e.g., the cryosphere, chemistry and biosphere. In addition, the decision must be made about whether computational resources should go towards increased horizontal, vertical and temporal resolution or additional ensemble members.

Additional challenges are posed by intrinsically coupled phenomena like the Madden-Julian Oscillation (MJO) and tropical cyclones. These – in origin tropical processes - are multi-scale processes that need to resolve small-scale processes such as convection in addition to capturing the large-scale ocean response and feedback. Many of the Coupled Model Intercomparison Project phase 5 (CMIP5) climate models still do not properly simulate the MJO and convectively coupled waves (Hung et al., 2013).

Rigorous mathematical methods exist for dealing with the construction of parameterizations – usually referred to as the operation of coarse graining and performed through the method of homogenization (Papanicolaou and Kohler 1974; Gardiner 1985; Arnold, 1992) - when there is a vast time scale separation between the portion of the system we are interested in describing and the fast processes we want to represent in a simplified manner. Note that, typically, a relationship can be found between spatial and temporal scales of variability, with fast processes associated to small scales and slow processes associated to large scales, so that separating physical processes by timescales often results in decomposing small scale features from large scale phenomena.

Mathematical approaches to stochastic modeling rely on the assumption that a physical system can be expressed in terms of variables of interest, and variables which one does not want to explicitly resolve. The goal is then to derive an effective equation for the slow predictable processes and to represent the effect of the now unresolved variables as random noise term. Such a thinking underlies the pioneering study of Hasselmann (1976), who split the coupled ocean-atmosphere system into a slow ocean and fast weather fluctuation components and subsequently derived an effective equation for the ocean circulation only. One finds that the impact of the fast variables on the dynamics of the slow variables boils down to a deterministic correction – a mean field effect sometimes referred to as noise-induced drift or rectification – plus a stochastic component, which is a white random noise in the limit of infinite time scale separation. The advantage of such a rigorous approach is that all parameterizations are valid for increasing spatial resolutions ("scale-aware parameterizations"), which is an important aspect in developing seamless and multi-resolution prediction models.

The time scale separation does not necessarily require a gap in the power spectrum of the coupled process, however, it assumes that the decorrelation time of the fluctuating processes is sufficiently smaller than the decorrelation time of the slow processes (e.g., Gardiner, 1985). An example for a simple red noise model that has time scale separation in this sense, but not a gap in the power spectrum is e.g., discussed in DelSole (2000).

The condition of scale separation is unfortunately not met in typical geophysical fluid dynamics applications. Statistical mechanics – and in particular the Mori-Zwanzig theory (see e.g. Zwanzig 2001) – says that when the time scale separation between the fast and slow processes is not too large, the picture of the parameterization as being constructed as the sum of a suitably defined deterministic plus random corrections has to be amended to take memory effects into account (Wouters and Lucarini (2012, 2013), Chekroun et al. 2015a, 2015b). As a result, a great challenge is posed by the representation of partially resolved processes. For example, climate models and even many weather models split the fundamental process of convection into a resolved (large-scale) and parameterized component (e.g. Arakawa, 2004). The range of scales on which a physical process is only partially resolved is often called the "gray zone" (e.g., Gerard, 2007). The equilibrium assumption no longer holds (e.g., Yano and Plant, 2012a,b) and the subgrid-scale parameterization takes a prognostic form rather than being diagnostic, as explicitly shown by Yano (2014) for mass-flux formulation. As the next generation of numerical models attempts to seamlessly predict weather as well as climate, there is an increasing need to develop parameterizations that adapt automatically to different spatial scales ("scale-aware parameterizations").

Reviews of rigorous mathematical approaches to stochastic parameterizations that are accessible to wide audiences are available (Penland 2003a,b, Majda et al., 2008, Franzke et al. 2015). Different from these articles, the focus here is to report on successful applications of stochastic parameterizations to pressing questions in the atmospheric sciences.

Stochastic parameterization schemes are now routinely used by operational weather and climate centers to make ensemble predictions from short-range to seasonal time scales (e.g., Texeira et al., 2008, Berner et al. 2009, Palmer et al. 2009, Palmer, 2012, Sanchez et al. 2015, Suselj et. al. 2013, 2014, Weisheimer et al. 2014). The most common stochastic parameterization schemes employed are the stochastically perturbed parameterization tendencies (Buizza et al., 1999; Palmer et al., 2009; Berner et al. 2015, Weisheimer et al. 2014) and the stochastic kinetic-energy backscatter scheme (Shutts, 2005; Berner et al., 2008, 2009, 2011, 2015; Tennant et al. 2011, Romine et al., 2015). In these applications, underdispersive ensemble systems tend to produce over-confident and, thus, unreliable forecasts. Stochastic perturbations increase the diversity between ensemble members, which results in a more reliable and thus skillful ensemble system. Since the stochastic schemes are designed to mimic processes that are either unresolved or altogether unrepresented, they are often referred to as *model-error schemes*. Alternative approaches that fall under this category, but are not stochastic, are e.g. multi-physics schemes, which use different physical parameterization packages for each ensemble member.

Previous reviews of stochastic approaches applied to atmospheric and oceanic models are available e.g., in Palmer 2001; Palmer and Williams 2008, Williams et al. 2013. This body of work identifies the assessment of the benefits of stochastic closure schemes compared to their more conventional deterministic counterparts as a key outstanding challenge in the area of mathematics applied to the climate system. Palmer (2012) argues that well-designed stochastic climate ensembles are better suited to estimate the true uncertainty in climate predictions than current *ad hoc* poor-man ensembles, produced by combining forecasts from different climate centers.

A fundamental argument, that has been often overlooked, is that merits of stochastic parameterization go far beyond providing uncertainty estimations for weather and climate predictions, but are also needed for better representing the mean state (e.g., Sardeshmukh et al., 2001; Palmer, 2001, Penland 2003a,b; Berner et al. 2012, Weisheimer et al. 2014) and regime transitions (e.g., Williams et al. 2003, 2004; Birner and Williams 2008, Christensen et al. 2015a) via inherent non-linear processes. This is especially relevant for climate predictions, which have long-standing mean state errors, such as e.g., a double intra-tropical convergence zone (e.g., Lin et al, 2007), and erroneous stratocumulus cloud covers, which play a crucial role in the climate response to external forcing. Insofar as stochastic parameterizations can change the mean state, they have the potential to affect the response to changes in the external forcing (e.g., Seiffert and von Storch, 2008). Results from a more mathematic perspective consider, how the invariant measure of a deterministic dynamical system is affected by stochastic forcing (Lucarini, 2012) and how climate response can be framed as a problem of non-equilibrium statistical mechanics (Lucarini and Sarno 2011, Lucarini et al. 2014a). The impact of stochastic parameterization on the tail behavior of the resulting probability density has only very recently been considered (Sardeshmukh and Sura 2009, Sura 2011, Franzke 2012, Sardeshmukh et al.

2015, Tagle et al. 2015).

The essential fact that a white-noise forcing with zero mean can lead to a non-linear or rectified response and change the mean state is shown in Figure 1a-d. Assume the nonlinear climate system can be simplified as a double-well potential. If the noise is sufficiently small and under appropriate initial conditions, the system will stay in the deeper potential well and the associated probability density function of states will have a single maximum. As the amplitude of the noise increases, the system can undergo a noise-induced transition and reach the secondary potential well (e.g., Horsthemeke and Lefever, 1984). The resulting probability density function (PDF) will exhibit two local maxima, signifying two different climate regimes, rather than a single maximum, as in the small-noise scenario. Note, that the stochastic forcing not only increases the variance, but also the mean. But even a linear system characterized by a single potential can change the mean if forced by multiplicative or state-dependent white noise (Figure 1e-h). Noise is multiplicative, if its amplitude is a function of the state, which is denoted by the red errors of different length in Figure 1g. The noise-induced drift changes the mean state and can produce non-Gaussian PDFs (e.g. Berner, 2005, Berner et al. 2005, Sura et al. 2005)

Here, we argue, that stochastic parameterizations are equally essential for:

• the estimation of the uncertainty of weather and climate predictions,

• a reduction in systematic model errors,

• triggering noise-induced regime transitions,

• capturing the linear or non-linear response to changes in the external forcing, and should be applied in a systematic and consistent fashion, not only to weather, but also to climate simulations.

The paper is organized as follows: First we give examples of the successful routine use of stochastic parameterizations in weather and climate models. We then discuss recent developments in the field, where uncertainty is introduced within particular physical parameterizations based on expert knowledge. Subsequently, mathematical rigorous approaches to the parameterization problem are introduced and applications to weather and climate reviewed.

2 Representing Uncertainty in Comprehensive Climate and Weather Models

2.1 Adding uncertainty a posteriori: the stochastically perturbed parameterization tendency schemes and the stochastic kinetic-energy backscatter scheme

Stochastic parameterizations are based on the notion that – especially with increasing numerical resolution – the method of averaging (Arnold, 2001; Monahan and Culina 2011) is no longer valid and the subgrid-scale variability should be sampled rather than represented by the equilibrium mean.. In addition, certain subgrid-scale processes interact with larger scales, and due to the truncation, these interactions, with possibly large-scale impacts, are no longer represented.

The former is addressed by the stochastically perturbed parameterization tendency (SPPT) scheme, which multiplies the net tendencies of the physical process parameterizations (convection, radiation, cloud physics, turbulence and gravity wave drag) at each gridpoint and time step with multiplicative noise. One essential feature is that the noise is correlated in space and time. SPPT has a beneficial impact on medium range, seasonal and climate forecasts (Buizza et al., 1999; Palmer et al., 2009; Weisheimer et al. 2014; Christensen et al, 2015b; Dawson and Palmer, 2015), and Watson et al (2015) showed that the multiplicative SPPT scheme is consistent with observations of tropical convection as a function of the large-scale state.

The stochastic kinetic-energy backscatter scheme (SKEBS) aims to represent model uncertainty arising from unresolved subgrid-scale processes and their interactions with larger scales by introducing random perturbations to the streamfunction and potential temperature tendencies, i.e. the scheme re-injects a small fraction of the dissipated energy into the resolved scales, that then interacts with the resolved-scale flow. Originally developed in the context of Large-Eddy-Simulations (Mason and Thomson, 1992), and applied to models of intermediate complexity (Frederiksen and Davies, 1997), it was adapted by Shutts (2005) for Numerical Weather Prediction (NWP). Its beneficial impact on weather and climate forecasts are reported e.g., in Berner et al. (2008, 2009, 2011, 2012, 2015), Bowler et al. (2008, 2009); Palmer et al. (2009); Doblas- Reyes et al. (2009); Charron et al. (2010); Hacker et al. (2011); Tennant et al. (2011); Weisheimer et al. (2011,2014). A variant of SKEBS perturbs convective processes only (Shutts, 2015, Sanchez et al. 2015).

While these schemes are motivated by physical reasoning and the scheme parameters are informed by e.g. coarse-graining high-resolution output (Shutts and Palmer, 2007; Shutts and Callado Pallarès, 2014), the amplitude of the perturbations is often determined empirically by choosing a value that satisfactorily reduces the underdispersion. Obviously such an approach is only possible for forecast ranges where verification is possible, such as for short-term, medium-range and seasonal forecasts. A common criticism of this approach is that the improved skill is solely the result of an increase in reliability. However, Berner et al. (2015) found that the merits of model-error representations, stochastic or not, go beyond increasing reliability through increased spread and can account for structural model uncertainty.

In the following examples, we demonstrate that stochastic parameterization is able to improve the mean state representation as well as the variability. First, we present recent results from the seasonal forecasting system at ECMWF (System 4). Hindcast ensembles providing 7-month forecasts for the years 1981-2010 were started 4 times a year, both with and without stochastic perturbations (Weisheimer et al. 2014). The SPPT scheme helped to reduce excessively strong convective activity especially over the Maritime Continent and the tropical Western Pacific, leading to reduced biases of the outgoing longwave radiation (OLR), cloud cover, precipitation and near-surface winds (Figure 2). Positive impact of the stochastic schemes was also found for the statistics of the MJO, the dominant mode of sub-seasonal tropical variability, showing an increase in the frequencies and amplitudes of MJO events (Figure 3). A reduction of excessive amplitudes in westward propagating convectively coupled waves in simulations with an earlier model version and SKEBS was previously reported in Berner et al. 2012.

Another example for the complex response of the climate system is evident in the spectra of sea surface temperatures in the El Nino 3.4 region. Compared to HadISST observations, climate simulations with the Climate Earth System Model (CESM) run for a period of 135 years at a resolution of 1° (ca 100km) have three times more power for oscillations with periods between 2 to 4 years (Figure 4). In simulations with SPPT, the temperature variability in this frequency range is greatly reduced, leading to a much better agreement between the simulated and observed spectra (Christensen, Berner, Coleman and Palmer, manuscript in preparation).

Along with the improvements of the model climate in the tropics, the stochastic perturbations also benefit the forecast performance on seasonal timescales. With the stochastic schemes, the forecast errors of tropical Pacific SSTs are reduced, while increases in the ensemble spread lead to a more reliable ensemble system. This has been reported for forecasts with earlier versions of the ECMWF system (Berner at al., 2008; Dobles-Reyes et al. 2009; Palmer at al. 2009) and confirmed in recent integrations with System 4 (Weisheimer et al. 2014) and in the EC-Earth v3.0.1 Earth system model (Batté and Doblas-Reyes, 2015). For example, the perturbations from the SPPT scheme increase the ensemble spread in Nino 3.4 area sea-surface temperatures in a 5-member ensemble with the EC-Earth model (Figure 5). For a horizontal resolution of ca. 60km (T255) for the atmospheric and ca. 100km for the ocean component, SPPT leads to a significant decrease in the ensemble mean error.

A number of studies have found evidence for stochasticity leading to noise-induced transitions in mid-latitude circulation regimes, especially over the Pacific-North America region (Jung et al. 2005, Berner et al. 2012, Dawson et al. 2015, Weisheimer et al. 2014). These results support the idea that stochastic parameterizations might be relevant also for improving the representation and the predictive skill on low-frequency variability features.

2.2 Perturbed parameter approaches

Parameterizations of subgrid-scale processes contain closure assumptions, and related parameters with inherent uncertainties. Although increasing model resolution gradually pushes these assumptions further down the spectrum of motions, it is realistic to assume that some form of closure will be present in simulation models into the foreseeable future.

Parameter uncertainty can be pinpointed in ensemble prediction systems by so-called perturbed parameter schemes (e.g. Bowler et al., 2008), i.e. perturb the closure parameter(s) with a fixed value. For instance, Reynolds et al. (2011) included parameter perturbations to boundary-layer and convection schemes, and noted a positive impact on tropical ensemble spread and Brier scores in a global forecasting system. Several studies find multi-parameter approaches less beneficial than other model-error schemes, for both mesoscale prediction systems (Hacker et al., 2011, Berner et al., 2011) and monthly and seasonal forecasts of near-surface temperature (Weisheimer, et al., 2011). Another limitation of this approach is that the parameter uncertainty estimates are subjective, and information about parameter interdependencies is not included.

Nevertheless, reductions in mean forecast error due to a unified stochastic parameterization of boundary layers and shallow convection were significant enough that a stochastic "eddy-diffusivity/ mass-flux" parameterization was implemented in the operational Navy Global Environmental Model (NAVGEM) in 2013 (Suselj et al. 2014). Improvement in the representation of convectively driven boundary layers and coupling between boundary layers and cumulus regions was achieved by parameterizing vertical fluxes as a sum of an eddy-diffusivity part (Louis 1979) with a stochastic mass-flux scheme.

Recently, Christensen et al. (2015b) constructed fixed and stochastically varying perturbed parameter schemes for representing uncertainty in four convection closure parameters. The parameter perturbations were based on an objective covariance estimate of parameter uncertainty (Järvinen et al. 2012; Ollinaho et al, 2013). The spread of ensemble forecasts was improved using the two schemes, with a larger impact observed for the fixed perturbed parameter scheme. A reduction in bias was observed for some variables (e.g. U850), and there was a significant improvement in forecast skill compared to the operational system (Figure 6). However, the ensembles remained underdispersive, indicating that the perturbed parameter schemes did not capture all uncertainty in the convection scheme. Indeed, for forecast variables that are particularly sensitive to convection, the SPPT scheme outperformed the perturbed parameter approaches.

A number of studies propose the use of stochastic approaches for the parameterization of gravity waves (GWs), since the GW field produced by convection, mountains or fronts is only predictable in a statistical sense (e.g., Eckermann, 2011, Doyle et al. 2011). Field campaigns reveal that the GW field is very intermittent and often dominated by well-defined GW packets. These properties are well simulated by stochastic parameterization schemes for non-orographic GW of Lott et al. (2012), Lott and Guez (2013) and de la Cámara and Lott (2015), which stochastically sample the GW spectrum. Recently, de la Cámara et al. (2014) showed that the free parameters of this scheme can be constrained by the probability density function of the observed GW momentum flux.

The effect of perturbing the surface heat fluxes that couple atmosphere and land models, and in particular the variability associated with land surface heterogeneity in vegetation is investigated e.g. in Langan et al. (2014). Vegetation heterogeneity within a grid-box is represented as fractional areas of different plant functional types (PFTs) in land models. Although surface heat flux bulk formulations are applied to each PFT separately, conventional parameterization of grid-box land-atmosphere surface fluxes simply computes the area-weighted average of surface heat fluxes over the different PFTs within the grid box. The new stochastic parameterization

(Langan et al. 2014) retains this subgrid-scale variability among PFTs by sampling the contribution of each PFT to the grid box representative value from a two-parameter multivariate Dirichlet distribution at each model time-step, rather than using the constant area weights. With this stochastic parameterization ensemble simulations with a single column model version of the Community Earth System Model (CESM) reveal greater variability in grid-box surface heat fluxes and an increase in the variability of convective precipitation as well as larger extreme values (Figure 7).

Physical parameters of land surface models often have very large uncertainties and are not well constrained by observations. A recent study by MacLeod et al. (2015) introduced parameter perturbations to two key soil parameters, the hydraulic conductivity and the van-Genuchten α, and compared their impact with stochastic perturbations of the soil moisture tendencies in seasonal forecasts with the ECMWF coupled model. Both the perturbed parameter approach and the stochastic tendency perturbations improved the forecasts of extreme air temperature for the European heat wave of 2003, through better representation of negative soil moisture anomalies and upward sensible heat flux. This demonstrates the potential and also the need to include explicit formulations of uncertainties in land surface models.

A component of the coupled atmosphere-ocean system that may be particularly suited for stochastic parameterization is the air-sea fluxes across the sea surface. These air-sea fluxes of energy and momentum vary on a vast range of space and time scales, including scales that are too small or fast to be resolved explicitly by global climate models. For example, subgrid convective clouds in the atmosphere will cause subgrid fluctuations at the air-sea interface, in both the downward fresh water flux (through precipitation) and the downward short-wave solar radiation.

Williams (2012) demonstrates in an important case a general aspect mentioned before, namely how stochastic fluctuations in the air-sea buoyancy flux may modify the mean climate, even though the time-mean fluctuation is zero. The mechanism is studied in climate simulations with a comprehensive coupled general circulation model and involves changes to the oceanic mixed-layer depth, sea-surface temperature, atmospheric Hadley circulation, and fresh water flux. The impact of the stochastic perturbations on the climatological mean net upward water flux (evaporation minus precipitation) is displayed in Figure 8. In addition to the changes to the time-mean climate, El Nino Southern Oscillation (ENSO) variability was significantly increased. These findings suggest that the lack of representation of subgrid variability in air-sea fluxes may contribute to some of the biases exhibited by contemporary coupled climate models.

Non-zero effects of fluctuating air-sea fluxes can result from non-linear responses to fluctuations of opposite signs. Beena and von Storch (2009) discussed such a response to a fluctuating buoyancy flux. In regions where the ocean is mostly stable, an extremely large positive buoyancy flux anomaly will sustain the existing stratification. On the contrary, an extremely large negative buoyancy anomaly can make the water column unstable, thereby triggering convective events that significantly alter the existing stratification.

Juricke et al. (2013) and Juricke and Jung (2014) recently investigated the sensitivity of an ocean-sea ice model and a coupled ocean-sea ice/atmosphere model to variations in the ice strength parameter. Sea ice rheology is a highly non-linear parameterized process of great importance for modeling sea ice drift and is sensitive to the amplitude of the ice strength parameter. As this parameter is not observable and is generally taken to be constant in time and space, large uncertainties remain in the choice of its value. Varying this parameter stochastically results in changes to the mean sea ice distribution as well as sea ice spread. In a coupled model, Juricke et al. (2014) compare the ensemble spread generated by atmospheric initial perturbations only to that generated by additional stochastic ice strength perturbations. Especially in the first few weeks of the forecast, incorporation of stochastic ice strength perturbations leads to considerably more sea ice spread in the central Arctic (Figure 9), which better reflects the forecast uncertainty.

Li and von Storch (2013) demonstrate the necessity of stochastic perturbations in ocean models and for ocean-atmosphere interactions. This study investigates the validity of stochastically representing mesoscale eddies in the ocean. Differently from the atmospheric case, oceanic mesoscale eddies in state-of-the art ocean models are normally not resolved, because of the small oceanic Rossby deformation radius. So far, the main effort has been on the parameterization of the mean effect of these eddies, e.g. via the Gent-McWilliams scheme (Gent and McWilliams, 1990). To see whether it is justified to replace the classical eddy parameterization by a stochastic parameterization that takes fluctuations into account, Li and von Storch (2013) quantified the total eddy forcing, defined as the divergence of eddy flux, in a simulation performed with a 1/10-degree ocean model. The magnitude of the fluctuating component of this forcing is about one order of magnitude larger than the mean component of this forcing (Figure 10) suggesting that classical eddy parameterization based on the mean field should indeed be replaced by a parameterization that takes fluctuating fluxes into account. Future work will aim at a stochastic parameterization of the fluctuating subgrid-scale eddies.

3. Systematic mathematical and statistical physics approaches

This section introduces systematic mathematical and statistical approaches to the parameterization problem and reports on recent work on the application of these rigorous methods to the weather and climate system.

3.1. The Stochastic Primitive Equations

Although the motions of the atmosphere and ocean are described by the Navier-Stokes equations, large-scale numerical models use the deterministic primitive equations (i.e. apply the hydrostatic approximation) in their dynamical core. An important advance is thus the derivation of stochastic primitive equations during the last decade: at first for two-dimensional flows (Ewald et al. 2007; Glatt-Holtz and Ziane 2008; Glatt-Holtz and Temam 2011) and recently for the full three-dimensional setting (Debussche et al. 2012).

While it is important to have rigorous underpinnings of the stochastic primitive equations, it is also important to understand that stochastic systems require numerical schemes fundamentally different from the ones available to solve deterministic systems. The reason for this is the irregularity of the paths of stochastic processes, which leads to integration methods different from the Lebesgue-integrals for deterministic systems (see Gardiner 2009 for an accessible text book). The two most commonly used stochastic integral types are the Itô-integral (Itô, 1951) and the Stratonovich-integral (Stratonovich, 1966). Which of the two integration types is appropriate depends on the stochastic properties of the physical system.

Starting in the 1970s a solid framework of numerical methods for stochastic ordinary differential equations was developed (Rümelin 1982; Kloeden and Platen 1992; Milstein 1995; Kloeden 2002). However, the development of high-order numerical schemes for stochastic partial differential equations remains an elusive task. Recently, there has been a breakthrough by Jentzen and Kloeden (2009); and by Weniger (2014) who proved the strong convergence of a Galerkin approximation for the three-dimensional stochastic primitive equations. With stochastic parameterizations becoming very common in weather and climate simulations, a revision of the deterministic numerical schemes should be undertaken to ensure the convergence of the numerical solutions for stochastic models.

3.2. Mathematically rigorous representation of unresolved degrees of freedom

Numerical weather and climate modeling can be seen as a model reduction problem. Because we cannot numerically solve the full continuous equations we have to truncate the equations at some scale and then treat the unresolved processes in some smart way. A systematic approach for the derivation of reduced order models from first principles is by adiabatic elimination (Gardiner 2009) or the stochastic mode reduction (Majda et al. 1999, 2008, Franzke et al. 2015). Proposed by Wong and Zakai (1965), Khas'minskii (1966), Kurtz (1973), Papanicolaou and Kohler (1974) and Papanicolaou (1976), method was expanded and successfully applied to a hierarchy of climate models by Majda et al. (1999, 2001, 2003, 2008), Franzke et al. (2005) and Franzke and Majda (2006).

In the stochastic mode reduction, the state vector is decomposed into slow and fast components, assuming timescale separation in the decorrelation time of these processes. Furthermore, it is assumed that the nonlinear self-interaction of the fast modes can be represented by a stochastic process. Under these assumptions an effective equation for the slow modes can be derived analytically (Majda et al. 2001). The stochastic mode reduction has been demonstrated to successfully model regime-behavior and low-frequency variability in conceptual models of the atmosphere (Majda et al., 2003), the barotropic vorticity equation on the sphere with realistic topography (Franzke et al. 2005) and a quasigeostrophic three-layer model on the sphere with realistic orography (Franzke and Majda, 2006). Geostrophically balanced models like those inevitably lead to a stochastic parameterization where all resolved degrees of freedom are coupled directly. For more comprehensive models this would put insurmountable demands to computer memory. Dolaptchiev et al. (2013 a,b), however, have successfully applied the stochastic mode reduction locally in the turbulent Burgers equations, potentially allowing the use of this method in full-scale climate models.

The stochastic mode reduction technique is rigorously valid only in the limit of large time-scale separation, though Dozier and Tappert (1978a,b), Majda et al. (2003, 2008), Franzke et al (2005) and Franzke and Majda (2006) showed empirically that the stochastic mode reduction can also work in situations with only moderate or no time scale separation. However, this poses limitations when constructing scale-aware parameterizations, where typically no separation exists (Sardeshmukh and Penland, 2015, Yano 2015, Yano et al. 2015). A potential solution to this problem was proposed by Wouters and Lucarini (2012, 2013) who analyzed a general two-level system (resolved and unresolved processes). Without making any assumption on the time scale separation between the two levels, but assuming instead the presence of weak coupling, Wouters and Lucarini found an explicit formulation for the parameterization of the impact of the unresolved variables, Y, on the resolved variables of interest, X. The first order term describes the mean field effect and corresponds to the deterministic parameterization (Figure 11a). The second order expansion includes two terms, one (Figure 11b).describing the impact of the fluctuations of the Y variables and leads to a rather general form of stochastic parameterization, the second term (Figure 11c). related to the memory effects and introducing non-Markovian properties to the dynamics. In the limit of infinite time scale separation between the two levels, the memory term can be neglected and the stochastic parameterization can be represented as a white noise forcing (as in the stochastic mode reduction).

The question of which stochastic process is best suited to describe the nonlinear interactions of the unresolved processes is an open question. While methods for Gaussian diffusion processes are well known (Oppenheim 1975, Gardiner 2009) it may be the case that other formulations like Lévy processes are better suited to describe the underlying physics (Penland and Ewald 2008, Penland and Sardeshmukh 2012; Hein et al. 2010; Gairing and Imkeller 2012, 2013; Thompson et al. 2015).).

3. 3 Adaptation of Concepts from Statistical Mechanics to Weather and Climate

A novel subgrid parameterization approach involves the adaptation of concepts from statistical mechanics to represent the subgrid-fluctuations. This is especially attractive for variable-resolution grids, since the statistics automatically adapt to the grid-resolution. Starting from the Gibbs canonical ensemble theory, Craig and Cohen (2006) developed a theory for the fluctuations in an ensemble of deep convective clouds. . Based on this theory, a stochastic parameterization of deep convection was developed to represent fluctuations of the subgrid convective mass flux about statistical equilibrium (Plant and Craig, 2008). To set a path towards the parameterization of fluctuations in a shallow convective cloud ensemble, the formalism of Craig and Cohen (2006) is generalized by introducing the influence of memory carried by the individual clouds on the ensemble statistics (Sakradzija et al., 2015). In a stationary shallow-convective cloud field, the cloud mass flux distribution deviates from an exponential distribution due to the correlation between the cloud mass fluxes and cloud lifetimes. This introduces a memory effect, which is more pronounced in a shallow convective ensemble because of the vast diversity in the shallow cloud life cycles (Sakradzija et al., 2015). Thus, the observed shallow convective variability can be reproduced across the different model scales using a formulation similar to Plant and Craig (2008) if the individual cloud memory is accounted for through the cloud-base mass flux distribution and by modeling the cloud life-cycles explicitly (Figure 12). This is an interesting example of the impact of the lack of time scale separation between the various dynamical processes in creating memory effects, discussed in general terms in Wouters and Lucarini (2012, 2013).

3.4 Discrete Processes and Data-driven methods

A recently introduced approach for stochastic convection parameterization represents the convective state (or the convective area fraction) of a model column as a discrete stochastic process. Only a few distinct convective states are possible, and the random transitions from one state to another as time evolves are modeled as a Markov chain. For example, Khouider et al. (2010) distinguish between 4 convective states or cloud states (clear sky, congestus, deep convection or stratiform), and Dorrestijn et al. (2013a) include an additional fifth state (shallow). The horizontal spatial domain of an atmosphere model is covered with a high-resolution lattice (with typical lattice spacing of 100m to 1000m), and on each lattice node lives a copy of this discrete stochastic process for the convective state (Figure 13). By averaging over blocks of lattice nodes, convective area fractions and related quantities can be obtained for spatial domains of arbitrary size. These fractions evolve randomly, and can be used as a basis for stochastic convection parameterization. Alternatively, such discrete stochastic processes can be used at a larger spatial scale, so that the discrete state represents convection over a much larger spatial domain, see e.g. Dorrestijn et al. (2013b) and Gottwald et al. (2015).

The probabilities for transitions between the convective states can be obtained in different ways. Dorrestijn et al. (2013a, b, 2015) and Gottwald et al. (2015) rely on statistical inference, following a procedure proposed by Crommelin and Vanden-Eijnden (2008). They use various datasets from convection-resolving Large Eddy Simulation or from observations. Khouider et al. (2010) and Frenkel et al. (2012) use physical insight to formulate transition probabilities for the Markov chain model. Although the restriction to a few convective states may seem crude, the resulting patterns and temporal behavior of the area fractions can be quite realistic. Furthermore, the formulation on a high-resolution lattice (or microlattice) makes it possible to compute convective fractions for varying area sizes, so that a parameterization based on these fractions can be scale-adaptive.

3.5 Fluctuation-dissipation theorem

Another statistical physics approach is offered by the fluctuation-dissipation theorem (FDT, Kubo 1966; Deker and Haake 1975, Hänggi and Thomas 1977; Risken 1984). Roughly speaking, in a large class of physical situations, the FDT relates the natural fluctuations of a system to its response to external forcing (Gritsun and Branstator 2007, Gritsun et al. 2008, Ragone et al. 2014). The FDT can be used to predict the response of objectively tuned parameters of subgrid-scale parameterizations. Achatz et al. (2013) have shown that this technique yields a better response with regard to the climate mean and variance than either a low-order model without changed parameters or the direct application of the FDT to predict these responses (Figure 14).

While FDT-based approaches have indeed had a certain degree of success in climate studies, a word of caution is necessary. One needs to underline that the FDT does not apply rigorously to an idealized non-equilibrium chaotic deterministic systems, because of the geometrical strangeness of the attractor, see Ruelle (2009). Nonetheless, prediction of climate response is still a treatable problem of statistical mechanics using a more general formulation of response theory (Lucarini and Sarno, 2011, Wouters and Lucarini 2013, Lucarini et al. 2014a, and Ragone et al. 2015). It is worth mentioning that including stochastic perturbations to the system leads to a smoothing of the invariant measure, which, in turn, makes the applicability of the FDT rigorously correct.

Further, in an intrinsically multiscale system like the climate, as discussed above, noise is unavoidably present as a result of the unresolved energy coupling and exchange processes occurring at very small temporal and spatial scales. Therefore, one expects that at all practical levels the invariant measure is indeed smooth (see textbooks by Gaspard 1998, Dorfman 1999, and references therein; see also Wouters and Lucarini 2013), and the application of stochastic Navier-Stokes equations (Landau and Lifschitz 1959; García and Penland 1991; Español 1998) seems well justified.

Seiffert and von Storch (2008) study the response of the climate system to CO2-forcing in the presence of small-scale fluctuations. This study demonstrated that the strength of the global warming due to a CO2-doubling depends on the representation of small-scale fluctuations and can be altered by up to 15% near the surface and up to 25% in the upper troposphere (Figure 15). Applying a stochastic model to their simulations, they found that the small-scale fluctuations change the temperature response via a statistical damping that acts as a restoring force. In addition, the small-scale fluctuations can affect feedback and interaction processes that are directly coupled to a CO2 increase, thereby altering the CO2-related radiative forcing (Seiffert and von Storch, 2010).

3.6 Renormalized closure parameterizations

A systematic approach to the self-consistent modeling of subgrid processes are renormalized closure parameterizations (Frederiksen and Davies 1997), which can be scale-aware (Frederiksen et al. 1996). Implementation of this approach into an atmospheric GCM resulted in significantly improved circulation and energy spectra (Frederiksen et al. 2003). Improved subgrid-scale parameterizations based on renormalized closure ideas were formulated and tested by Frederiksen (1999, 2012a,b), O'Kane and Frederiksen (2008), and Zidikheri and Frederiksen (2009, 2010a,b). Frederiksen and Kepert (2006) then used the functional form of these closure approaches to develop a zero-parameter stochastic modeling approach, where the drain, backscatter and net eddy viscosities are determined from the subgrid statistics of higher resolution reference simulations. This is in contrast to typical approaches in which heuristic subgrid parameterizations are developed based on some physical hypothesis on the behavior of subgrid turbulence.

Recently, Kitsios et al. (2012, 2013) used the approach of Frederiksen and Kepert (2006) to determine the eddy viscosities from a series of reference atmospheric and oceanic simulations. The isotropized version of the subgrid eddy viscosities where then characterized by a set of scaling laws. Large Eddy Simulations with subgrid models defined by these scaling laws were able to reproduce the statistics of the high resolution reference simulations across all resolved scales **(**Figure 16**).** These scaling laws further enable the subgrid parameterizations to be utilized more widely as they remove the need to generate the subgrid coefficients from a reference simulation.

Concluding Remarks

In this article, we attempt to narrow the gap between the fields of geo-sciences models and applied mathematics in the development of stochastic parameterizations: on the one hand geo-scientists are often unaware of mathematically rigorous results that can aid in the development of physically relevant parameterizations; on the other hand mathematicians often do not know about open issues in scientific applications that might be mathematically tractable.

Over the last decade or two, increasing evidence has pointed to the potential of this approach, albeit applied in an *ad hoc* manner and tuned to specific applications. This is apparent in the choices made at operational weather centers, where stochastic parameterization schemes are now routinely used to represent model inadequacy better and improve probabilistic forecast skill. Here, we revisit recent work that demonstrates that stochastic parameterization are not only essential for the estimation of the uncertainty in weather forecasts, but are also necessary for accurate climate and climate change projections. Stochastic parameterizations have the potential to reduce systematic model errors, trigger noise-induced regime transitions, and modify the linear or non-linear response to changes in the external forcing,

Ideally, stochastic parameterizations should be developed alongside the physical parameterization and dynamical core development and not tuned to yield a particular model performance, as is current practice. This approach is hampered by the fact that parameters in climate and weather are typically adjusted ("tuned") to yield the best mean state and/or the best variability. This can result in compensating model-errors, which pose a big challenge to model development in general, and stochastic parameterizations in particular. A stochastic parameterization might improve the model from a process perspective, but its decreased systematic error no longer compensates other model errors, resulting in an overall larger bias (Palmer and Weisheimer, 2011; Berner et al., 2012). Clearly, such structural uncertainties need to be addressed in order to improve the predictive skills of our models.

One exciting area that promises to deal with this issue is data assimilation, where the use of stochastic methods is already an active field of research. Stochastic methods have been shown to increase the spread in ensemble data assimilation, leading to a better match between observations and model forecasts and improved analyses (Isaksen et al. 2007, Mitchell and Gottwald, 2012, Ha et al. 2015, Romine at al. 2015). A cutting-edge frontier is the use of order moments and memory effects in Kalman filter data assimilation schemes (O'Kane and Frederiksen, 2012).

Mathematically rigorous approaches decompose the system-at-hand into slow and fast components. They focus on the accurate simulation of the large, predictable scales, while only the statistical properties of the small, unpredictable scales need to be captured. One finds that the impact of the fast variables on the dynamics of the slow variables boils down to a deterministic correction plus a stochastic component, which is a white random noise in the limit of infinite time scale separation (Arnold, 1992). This immediately points to the fact that the classical parameterization approach, which is only based upon averaged properties, is insufficient. Understanding the deterministic correction term in physical terms will shed light on the impact of stochastic parameterizations on systematic model errors and, hopefully, compensating model errors.

Recent findings from such rigorous derivations suggest that when the time scales of the processes we need to parameterize are not very different from those of the explicitly resolved dynamics – if we are in a grey zone - memory terms can become important (e.g., Wouters and Lucarini 2012, 2013; Chekroun et al. 2015a, 2015b). This is especially relevant for developing scale-aware parameterizations, where it is difficult to control the time scale separation as resolution is altered

The concepts underlying the mathematical systematic approach give raise to recent proposals regarding numerical approaches for multi-scale systems. Vanden-Eijnden et al. (2003) and Palmer (2014) argue that due to limited computational and energy power resources, only predictable scales should be solved accurately, while the smaller, unpredictable scales can be approximated on the fly.

It is our conviction, that basing stochastic parameterizations on sound mathematical and statistical concepts will lead to substantial improvements in our understanding of the Earth system as well as increased predictive capability in next generation weather and climate models.

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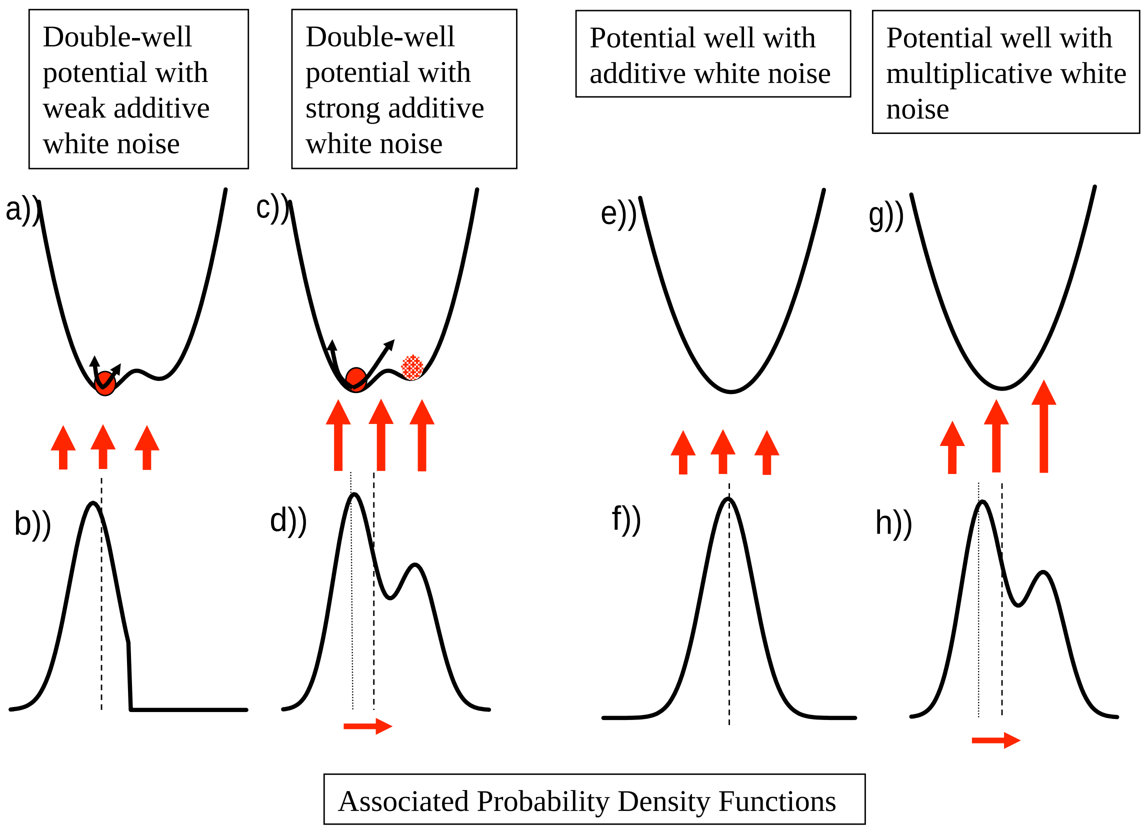

Figure 1: System characterized by a,c) double-potential or e,g) single-potential well and their associated probability density functions (PDFs). If the noise is sufficiently small (a) and under appropriate initial conditions, the system will stay in the deeper potential well and the associated probability density function of states will have a single maximum (b). As the amplitude of the noise increases, the system can undergo a noise-transition and reach the secondary minimum in the potential (c) leading to a shifted mean and increased variance in the associated probability density function (d). A linear system characterized by a single potential well and forced by additive white noise (e) will have a unimodal PDF. However, when forced by mutliplicative (state-dependent) white noise (g), the PDF can have multliple modes and a shifted mean (h).

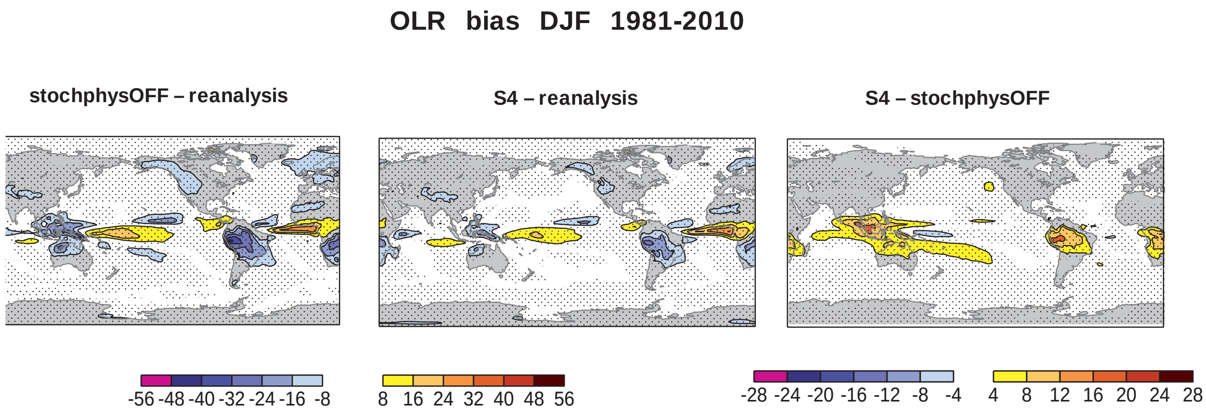

Figure 2: Top of the atmosphere net longwave radiation (outgoing longwave radiation; OLR) in W m–2 in DJF. Left: *stochphysOFF*–ERA-Interim reanalysis, middle: System 4–reanalysis, right: System 4 – *stochphysOFF*. Significant differences at the 95% confidence level based on a two-sided *t*-test are hatched. From Weisheimer et al. (2014).

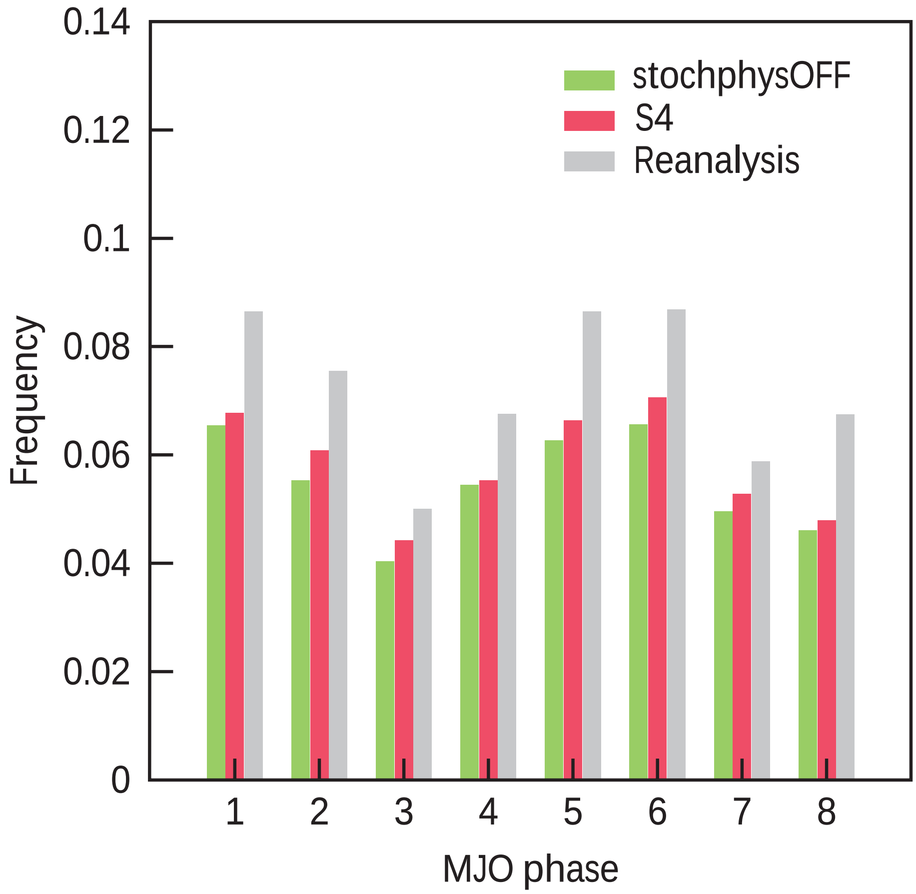

Figure 3: Relative frequencies of MJO events in each of the eight MJO phases. From Weisheimer et al. (2014).

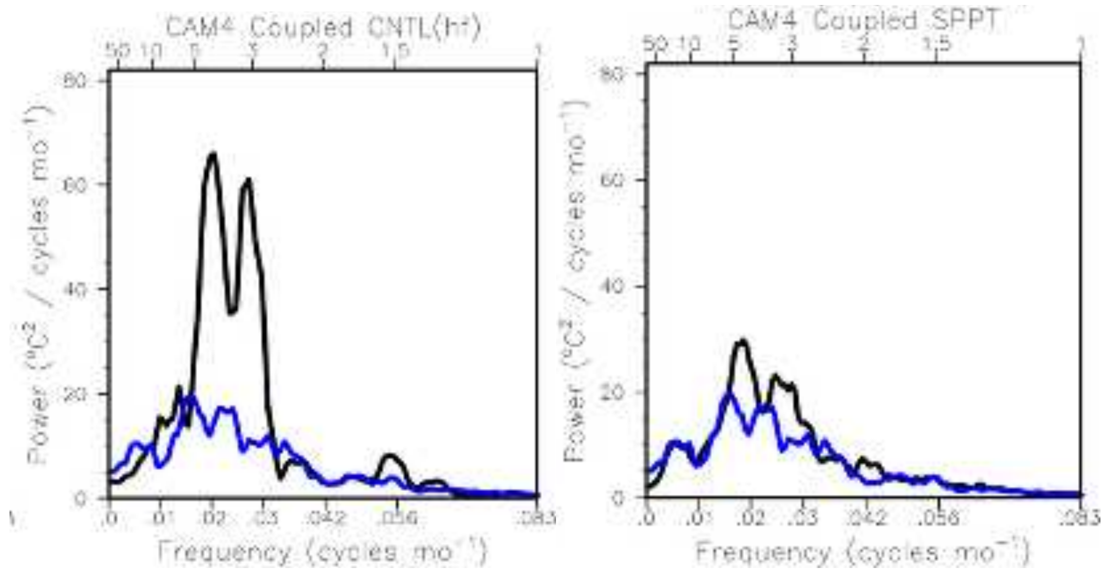

Figure 4: Power spectra of sea surface temperatures in El Nino 3.4 region in 135 year long simulations with the Community Earth System Model. Compared to HadISST observations (blue), the simulation has three times more power for oscillations with periods between 2 to 4 years (left). When the simulation is repeated with the stochastic parameterization SPPT, the temperature variability in this range is reduced, leading to a better agreement between the simulated and observed spectra (right).

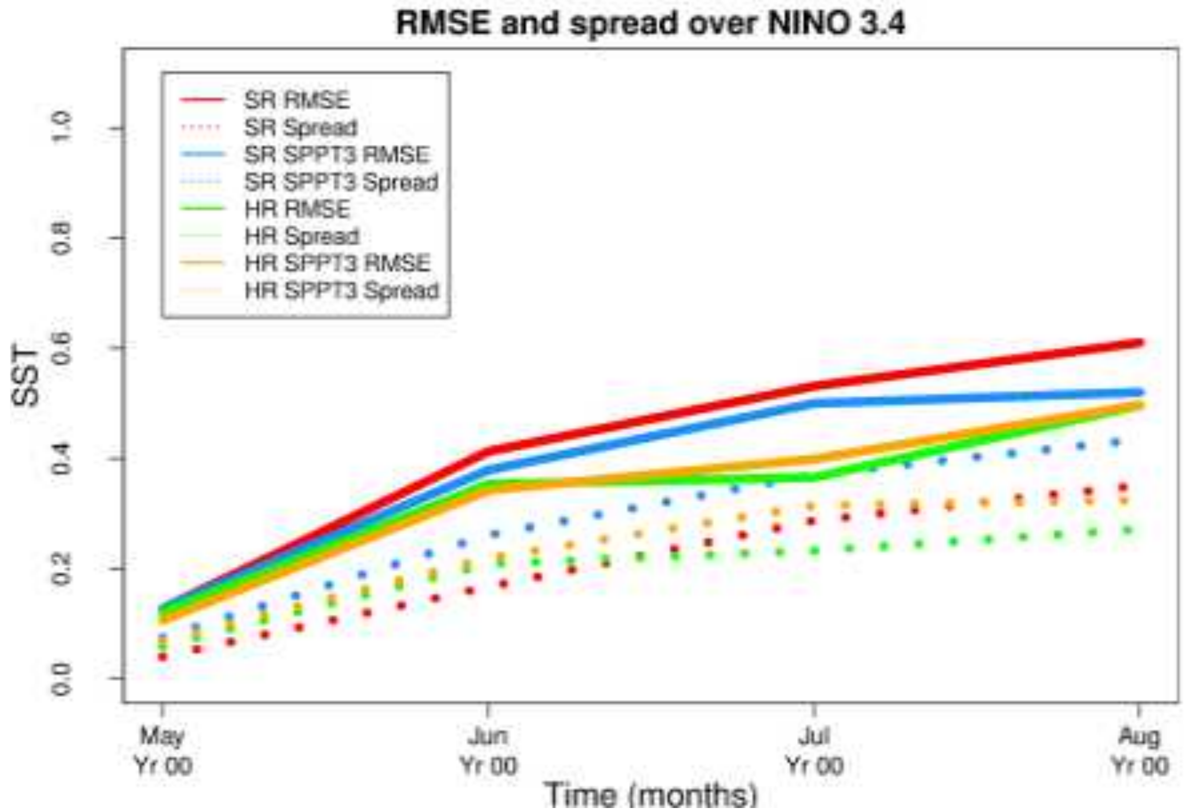

Figure 5: Niño 3.4 SST root mean square error (lines) and ensemble spread (dots) according to forecast time in EC-Earth 3 seasonal re-forecast experiments initialized in May 1993-2009 with standard (SR) or high resolution (HR) atmosphere and ocean components, with and without activating a 3-scale SPPT perturbation method in the atmosphere.

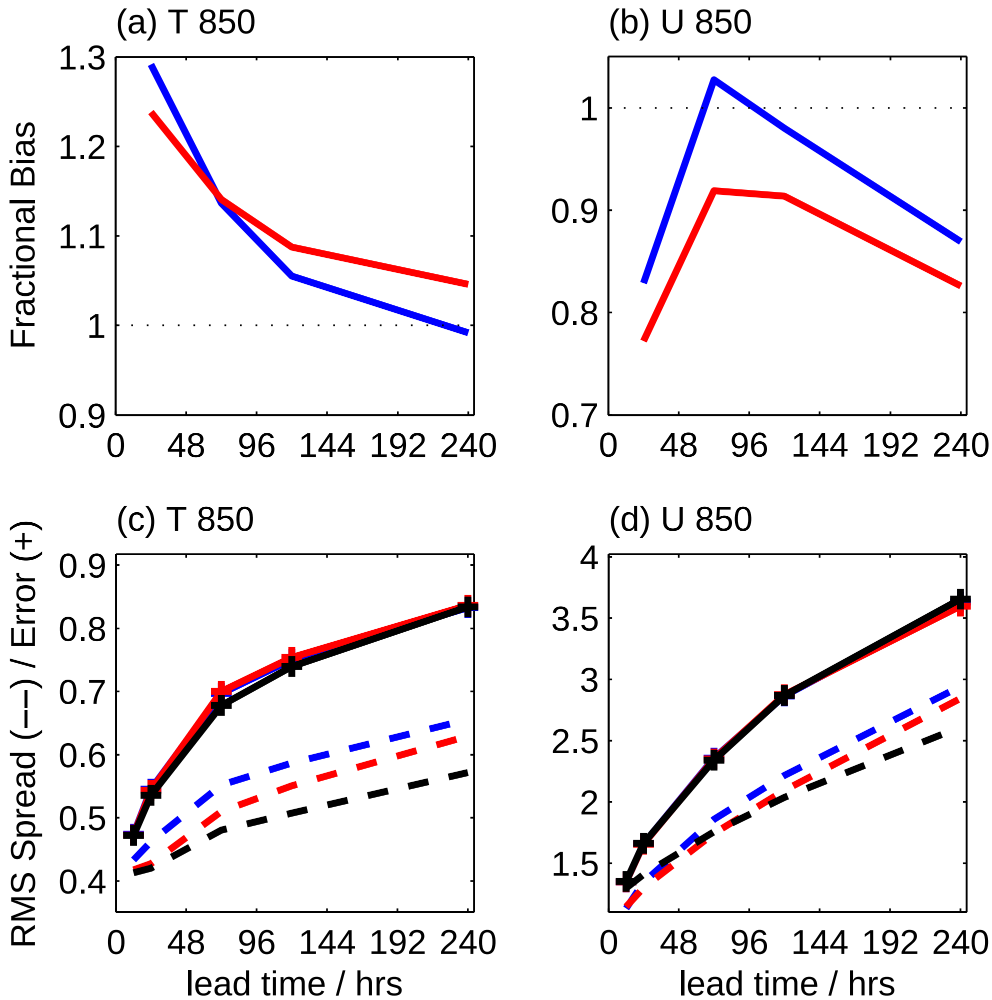

Figure 6: Forecast diagnostics as a function of time for the operational (black), fixed perturbed parameter (blue) and stochastically varying perturbed parameter (red) ensemble forecasts. Top: Forecast bias for (a) T850 and (b) U850 shown as a fraction of the bias for the operational system: BIAS /BIASoper. Bottom: Root mean square ensemble spread (dashed lines) and root mean square error (solid lines) for (c) T850 and (d) U850. Diagnostics are averaged over the region 10S-20N, 60-180E. Figure adapted from Christensen et al. (2015b).

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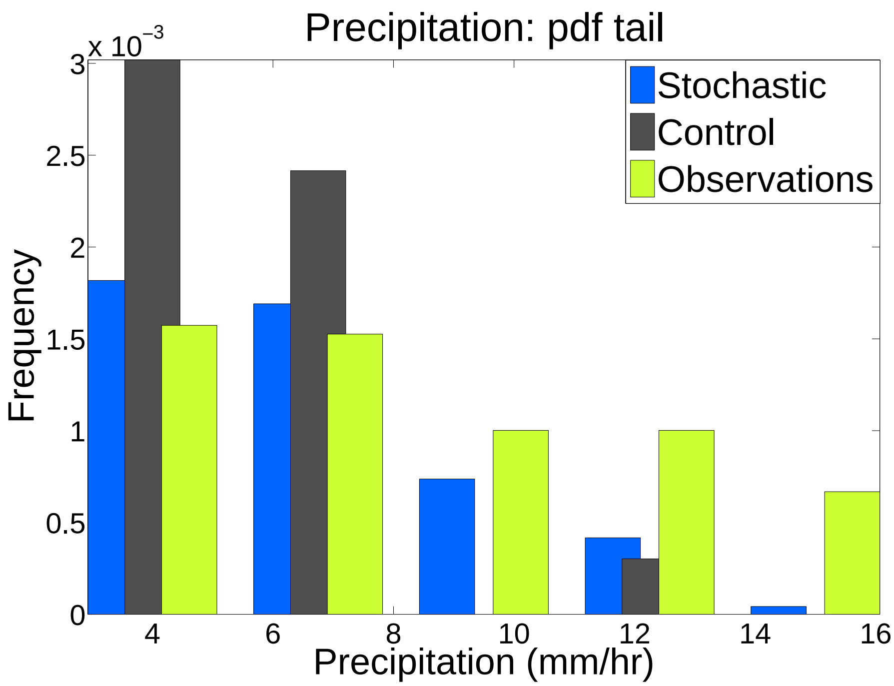

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Figure 7: The right tail of the probability density function of summer season hourly precipitation from a 50-member ensemble of one year single column model simulations with stochastic (blue) and conventional parameterizations (black) and fifteen years of observations (green) over a model grid box encompassing the US Department of Energy's (DOE) Atmospheric Radiation Measurement (ARM) program's site in Lamont, Oklahoma. The large-scale forcing for the single column model simulations are generated from a present day CESM simulation at a spatial resolution of about 2.8°x2.8°. From Langan et al. (2014).

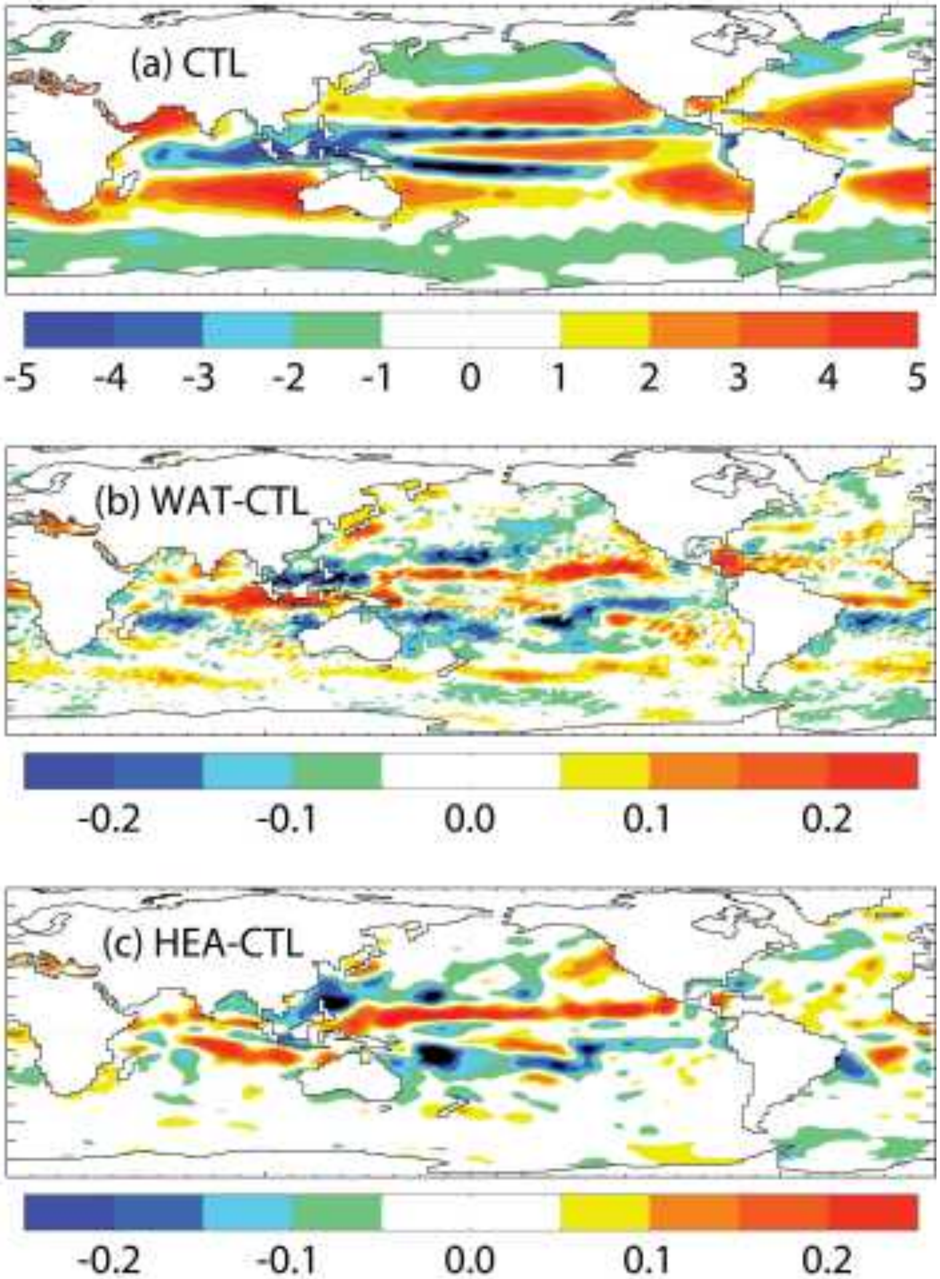


Figure 8: Maps of the century-mean net upward water flux (mm/day) at the sea surface in (a) CTL. (b) Difference from CTL for an experiments, where the net fresh water flux across the air–sea interface is stochastically perturbed before being passsed to the ocean. c) Difference from CTL for an experiment, where the net heat flux across the air–sea interface is stochastically perturbed before being passsed to the ocean. From Williams (2012).

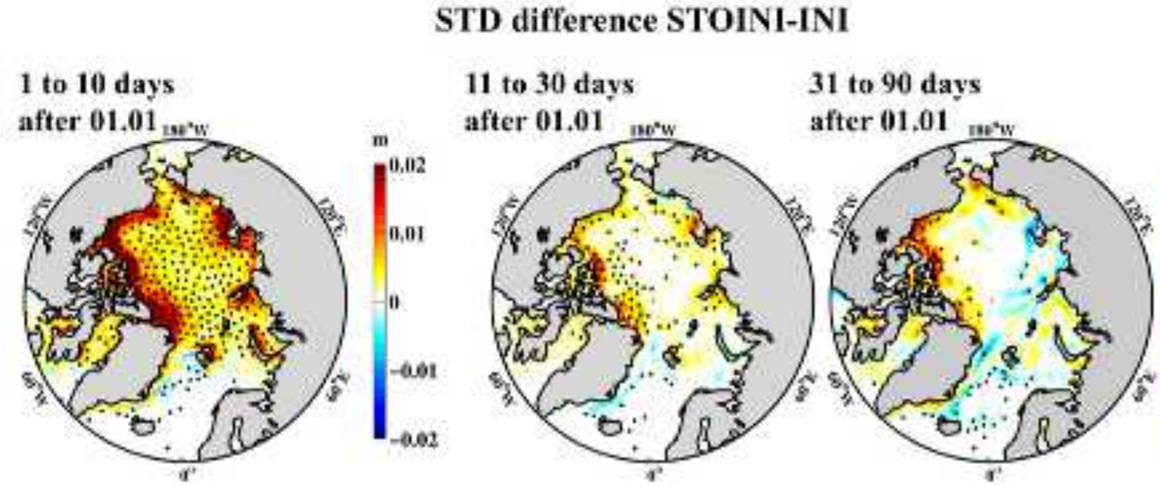


Figure 9: Difference in mean standard deviation of sea ice thickness forecasts (meters) between ensembles generated by stochastic ice strength as well as atmospheric initial perturbations (STOINI) and ensembles generated solely by atmospheric initial perturbations (INI), averaged for days (left) 1 to 10, (middle) 11 to 30, and (right) 31 to 90 after initialization at 00 UTC on 1 January. Stippled areas indicate differences statistically significant at the 5% level, using a two-tailed ***F*** test. Note the different contour intervals. From Juricke et al. (2014).

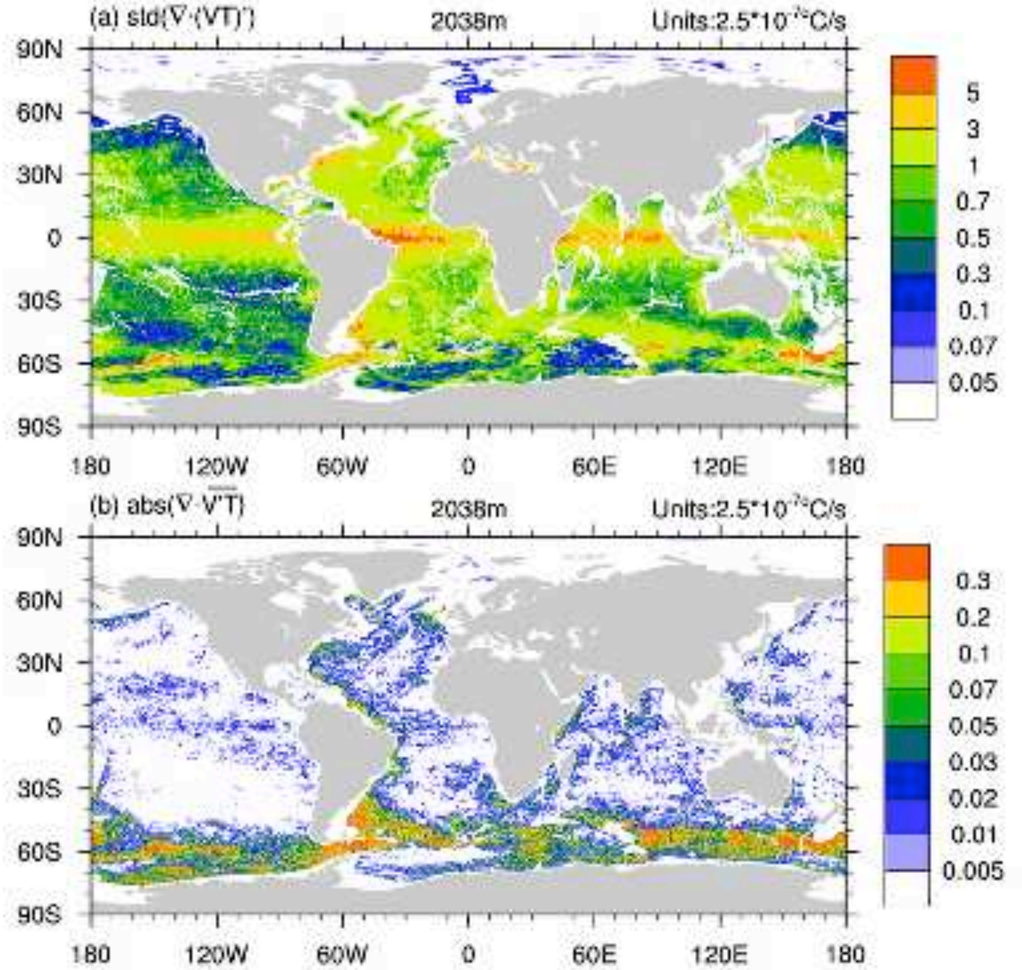
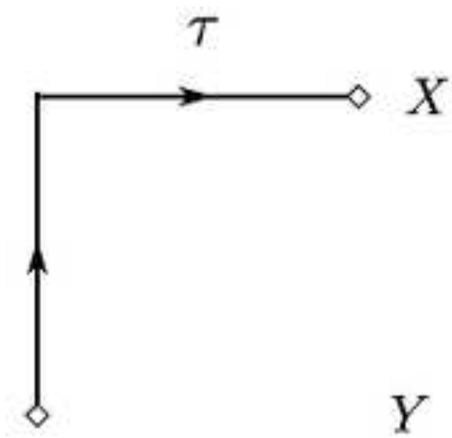
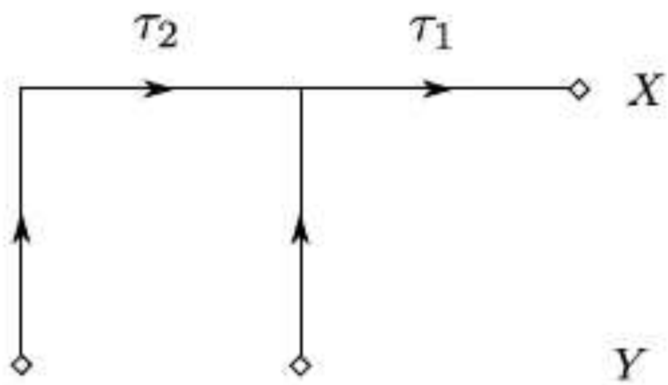


Figure 10: Top: Amplitude of fluctuations of the eddy forcing as measured by the standard deviation of divergence of eddy flux in a 1/10 degree OGCM. Bottom: Mean eddy forcing measured by the magnitude of the mean divergence of eddy heat flux in the same OCGCM.The amplitude of the fluctuations is about one order of magnitude larger than the mean eddy forcing. From Li and von Storch (2013).





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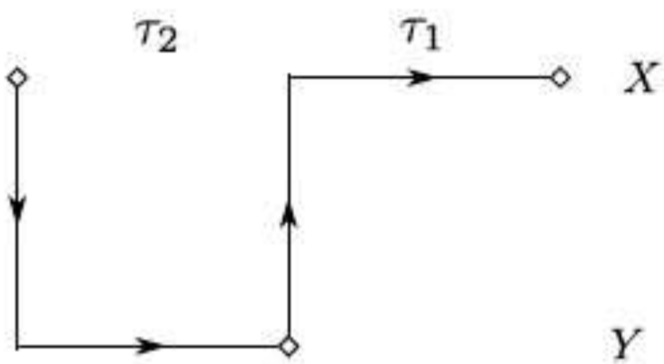

c)

Figure 11: Diagrammatic representation of the three terms contributing to the parameterization of the effect of the fast variables Y onto the dynamics of the slow variables X. a) First order contribution: average impact of the Y on the X variables.; corresponds to the deterministic mean field parameterization. b) Second order contribution: impact of the fluctuations of the Y on the X variables; corresponds to the stochastic parameterization. C) Secord order contribution: impact of the X variables on the X variables at a later time, mediated by the dynamics of the Y variables; corresponds to the memory effect.

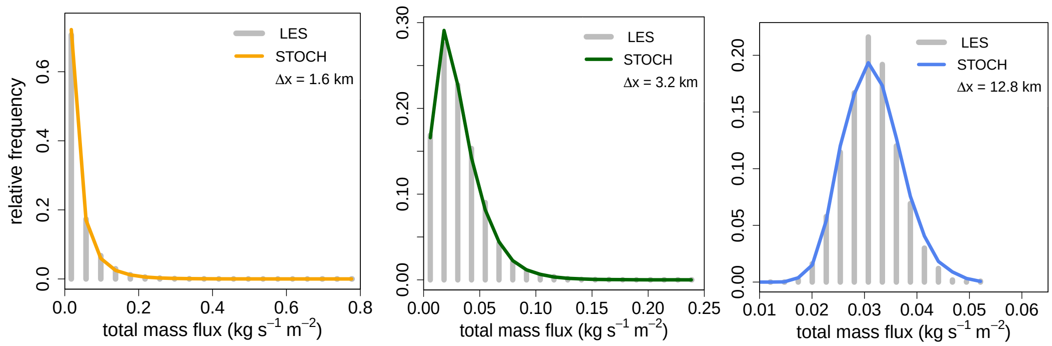

Figure 12: Histograms of the subgrid cloud-base mass flux, resulting from the stochastic shallow cumulus cloud scheme (STOCH) and coarse-grained large-eddy simulation (LES), are compared for three horizontal grid resolutions of 1.6 km, 3.2 km and 12.8 km. The stochastic scheme simulates a compound random process with the cloud number sampled from the Poisson distribution, while the individual cloud mass flux is sampled from a two-component mixed Weibull distribution. The histograms match closely and are scale-aware, which is an inherent property of the stochastic scheme, similar as in Plant and Craig (2008). From Sakradzija et al. (2015).

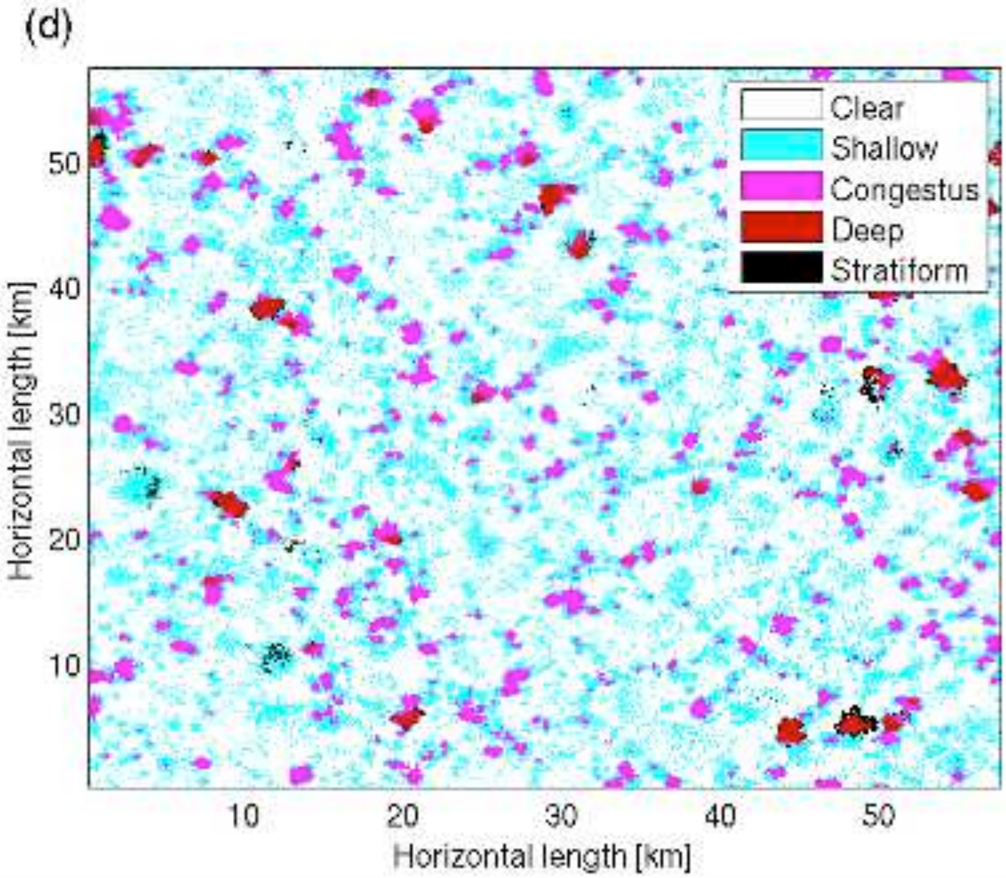

Figure 13: Snapshot of the spatial field of convective states obtained from Large Eddy Simulation data. The distinction between the various convective states was based on cloud top height and rainwater content. From Dorrestijn et al. (2013a).

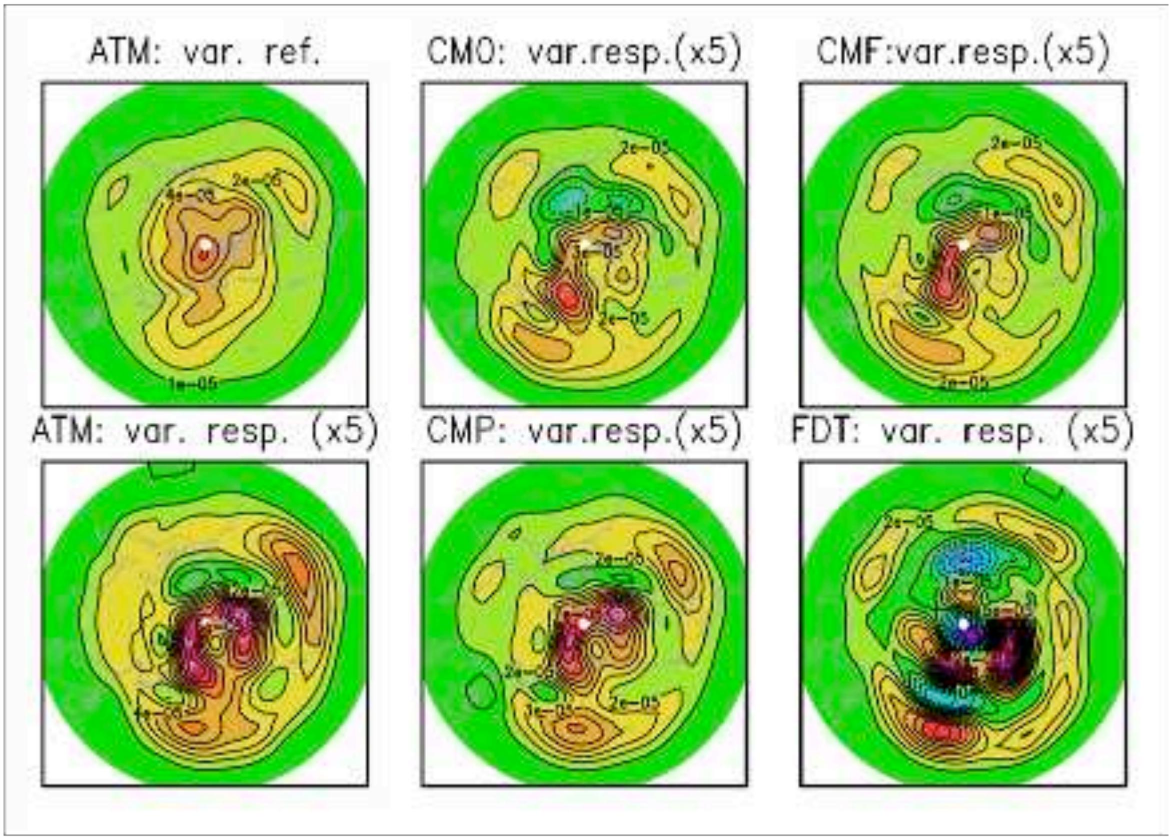

Figure 14: (Top left) The mean streamfunction variance of a barotropic-vorticity-equation model on the sphere, (bottom left) its response to an anomalous vorticity forcing at latitude 45N and longitude 210E, projected onto 90 EOFs, the simulation of this response (top middle) by a 90-EOF climate model with unmodified SGS parameterization (relative error 0.527), (bottom middle) by a climate model with SGS parameterization corrected a posteriori by investigation of the perturbed atmosphere, (top right) by a climate model with SGS parameterization corrected by FDT (relative error 0.342), and (bottom right) the direct estimation of the streamfunction-variance response by FDT (relative error 2.47). From Achatz et al. (2013).

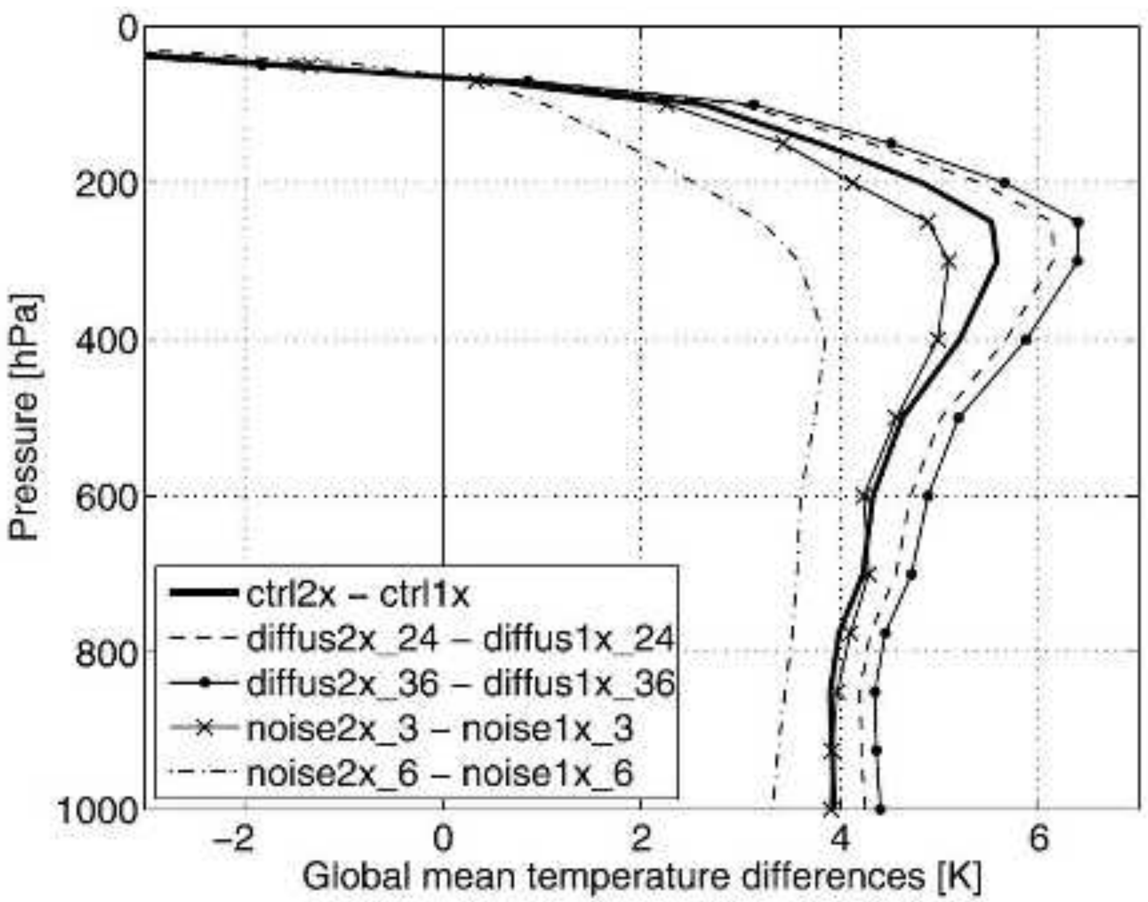

Figure 15: Climate responses of global mean temperature to a CO2 doubling (2x CO2 minus 1x CO2) obtained from the ECHAM5/MPIOM-experiments with different representations of small-scale fluctuations: 'diffus' refers to experiments in which the strength of horizontal diffusion is varied; 'noise' refers to experiments in which white noise is added to small scales of the atmospheric model ECHAM5. From Seiffert and von Storch (2008).

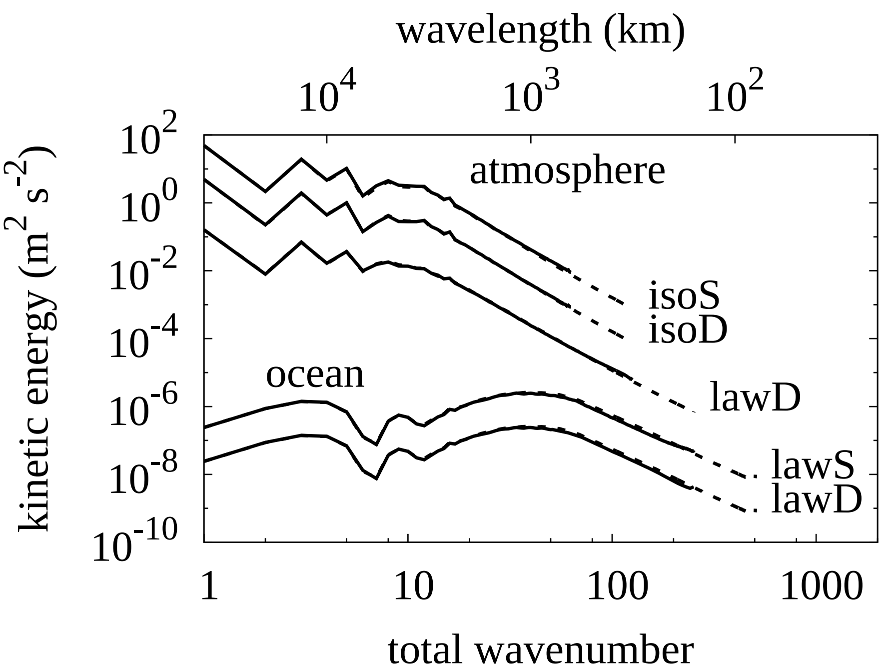

Figure 16: Top: Comparison of the upper level kinetic energy spectra of a two level benchmark simulation (dashed line) with associated LES (solid line) at various resolutions for: atmospheric isotropic stochastic (isoS) LES (top spectra); atmospheric isotropic deterministic (isoD) LES (second spectra); atmospheric deterministic scaling law (lawD) LES (third spectra); oceanic stochastic scaling law (lawS) LES (forth spectra); and oceanic deterministic scaling law LES (bottoms spectra).Top spectra has the correct kinetic energy, with the others shifted down for clarity. From Kitsios et al. (2014).