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

JUDITH BERNER*

National Center for Atmospheric Research+, Boulder, Colorado

ULRICH ACHATZ

Institut für Atmosphäre und Umwelt, Goethe-Universität, Frankfurt am Main, Germany

LAURIANE BATTÉ

CNRM-GAME, Météo-France/CNRS, Toulouse, France

LISA BENGTSSON

Swedish Meteorological and Hydrological Institute, Norrköping, Sweden

ALVARO DE LA CÁMARA

National Center for Atmospheric Research Boulder, Colorado

HANNAH M. CHRISTENSEN

University of Oxford, Atmospheric, Oceanic and Planetary Physics, Oxford

MATTEO COLANGELI

Gran Sasso Science Institute, Viale F. Crispi 7, 67100 L'Aquila, Italy

DANIELLE R. B. COLEMAN

National Center for Atmospheric Research+, Boulder, Colorado

DAAN CROMMELIN

CWI Amsterdam, the Netherlands and Korteweg-de Vries Institute for Mathematics, University of Amsterdam

* *Corresponding author address:* Judith Berner, NCAR, P.O.Box 3000, Boulder, CO 80303. E-mail: berner@ucar.edu

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STAMEN I. DOLAPTCHIEV

Institut für Atmosphäre und Umwelt, Goethe-Universität, Frankfurt am Main, Germany

CHRISTIAN L.E. FRANZKE

Meteorological Institute and Centre for Earth System Research and Sustainability (CEN), University of Hamburg, Hamburg, Germany

PETRA FRIEDERICHS

Meteorological Institute, University of Bonn, Germany

PETER IMKELLER

Institut für Mathematik, Humboldt-Universität zu Berlin, Berlin, Germany

HEIKKI JÄRVINEN

University of Helsinki, Department of Physics, Helsinki, Finland

STEPHAN JURICKE

University of Oxford, Atmospheric, Oceanic and Planetary Physics, Oxford

VASSILI KITSIOS

CSIRO Oceans and Atmosphere Flagship, 107-121 Station St, Aspendale, Victoria 3195, AUSTRALIA

FRANÇOIS LOTT

Laboratoire de Météorologie Dynamique (CNRS/IPSL), Ecole Normale Supérieure, Paris, France

VALERIO LUCARINI

Meteorological Institute Centre for Earth System Research and Sustainability (CEN), University of Hamburg, Hamburg, Germany; Department of Mathematics and Statistics, University of Reading, Reading, UK

SALIL MAHAJAN

Oak Ridge National Laboratory, USA

TIMOTHY N. PALMER

University of Oxford, Atmospheric, Oceanic and Planetary Physics, Oxford

CÉCILE PENLAND

Physical Sciences Division, NOAA/Earth System Research Laboratory, Boulder, Colorado

MIRJANA SAKRADZIJA

Max Planck Institute for Meteorology and Hans-Ertel Centre for Weather Research, Deutscher Wetterdienst, Hamburg, Germany

JIN-SONG VON STORCH

Max-Planck Institute for Meteorology, Hamburg

ANTJE WEISHEIMER

National Centre for Atmospheric Science (NCAS), University of Oxford, Atmospheric, Oceanic and Planetary Physics, Oxford, and ECMWF, Shinfield Park, Reading, UK

MICHAEL WENIGER

Meteorological Institute, University of Bonn, Germany

PAUL D. WILLIAMS

Department of Meteorology, University of Reading, Reading, UK

JUN-ICHI YANO

GAME-CNRM, CNRS, Météo-France, 42 Av. Coriolis, Toulouse, France

ABSTRACT

The last decade has seen the success of stochastic parameterizations in short-term, medium-range and seasonal forecasts: 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 better estimates of uncertainty, but it is also extremely promising for reducing longstanding climate biases and relevant for determining the climate response to external forcing.

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 the 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.

1 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 of geophysical fluid dynamics implies that many important physical processes (e.g. tropical convection, gravity wave drag, micro-physical processes) are still not resolved. Parameterizations of sub grid-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 or physical parameterization will be present in simulation models into the foreseeable future.

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 the cryosphere, chemistry and biosphere. In addition, the decision must be made about whether computational resources should go towards increased horizontal, vertical and temporal

111 resolution or additional ensemble members.

112 Additional challenges are posed by intrinsically coupled phenomena like the Madden-Julian
113 Oscillation (MJO) and tropical cyclones. Correctly simulating these tropical multi-scale
114 features requires resolving or accurately representing small-scale processes such as
115 convection in addition to capturing the large-scale response and feedback. Many of the
116 Coupled Model Intercomparison Project phase 5 (CMIP5) climate models still do not properly
117 simulate the MJO and convectively coupled waves (Hung et al. 2013).

118 A great challenge is posed by the representation of partially resolved processes (either in the
119 time or space domain). The range of scales on which a physical process is only partially
120 resolved is often referred to as the "gray zone" (e.g. Gerard 2007). In this gray zone, the number
121 of eddies in each grid box is no longer large enough to fulfill the "law of large numbers"
122 underlying deterministic bulk parameterizations and a stochastic approach becomes essential.
123 An example for a partially resolved process is convection, which is often split into a resolved
124 (large-scale) and parameterized component (e.g. Arakawa 2004). The equilibrium assumption
125 no longer holds when the model resolution is increased such that a clear scale separation
126 between convection and larger scales no longer is valid (e.g.Yano and Plant 2012a,b). In this
127 case the subgrid-scale parameterization takes a prognostic form rather than being diagnostic, as
128 explicitly shown for the mass-flux formulation by Yano (2014).

129 As the next generation of numerical models attempts to seamlessly predict weather as well as
130 climate, there is an increasing need to develop parameterizations that adapt automatically to
131 different spatial scales ("scale-aware parameterizations"). A big advantage of the
132 mathematically rigorous approach is that the subgrid-model is valid for increasing spatial
133 resolutions within a range of scales that is obtained as part of the derivation.

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. In the mathematical literature this is usually referred to as the operation of coarse-graining and performed through the method of homogenization (Papanicolaou and Kohler 1974, Gardiner 1985, Pavliotis and Stuart 2008). 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 terms.

Many stochastic parameterizations are based on the assumption of a scale separation between the temporal decorrelation rates between the rapidly fluctuating processes represented by a white noise and the slow processes of interest (e.g., Gardiner, 1985; Penland, 2003a). In geophysical applications, there is often - but not always – a relationship between spatial and temporal scales of variability, with fast processes associated with small scales and slow processes associated with large scales. If this is the case, separating physical processes by timescales can result in decomposing small-scale features from large-scale phenomena and spatial and temporal scale separation become equivalent.

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.

156 A simple example demonstrating noise-induced transitions and drifts is presented in Figure
157 1. Assume, the unforced nonlinear climate system can be described by a double-well
158 potential (a). If the noise is sufficiently small (denoted by short red arrows) and under
159 appropriate initial conditions, the system will stay in the deeper potential well and the
160 associated probability density function of states will have a single maximum (b). As the
161 amplitude of the noise increases (long arrows in c), the system can undergo a noise-induced
162 transition and reach the secondary potential well. The resulting probability density function
163 (PDF) will exhibit two local maxima (d), signifying two different climate regimes, rather
164 than a single maximum, as in the small-noise scenario. Note, that the stochastic forcing not
165 only changes the variance, but also the mean.

166 But even a linear system characterized by a single potential when unforced can change the
167 mean, if forced by multiplicative or state-dependent white noise (e-h). The noise is called
168 "multiplicative", if its amplitude is a function of the state, which is denoted by the red errors of
169 different length in panel g. The noise-induced drift changes the single-well potential of the
170 unforced system (e), so that the effective potential including the effects of the multiplicative
171 noise has multiple wells (not shown) and the associated PDF becomes bimodal (h). Note, that in
172 this example the shift in the mean compared to the unforced PDF (f) is caused by the noise,
173 which is referred to as "noise-induced drift" (see e.g., Sardeshmukh et al. 2001, Berner 2005,
174 Berner et al. 2005, Sura et al. 2005).

175 Operational weather and climate centers use now stochastic parameterization schemes routinely
176 to make ensemble predictions from short-range to seasonal time scales (e.g., Berner et al. 2009,
177 Weisheimer et al. 2014). Most ensembles suffer from underdispersion, which means that - on
178 average – the observed state is more often outside the cone of forecasts than can be statistically

179 justified. Stochastic perturbations introduce more diversity among the forecasts, which helps to
180 ameliorate this problem and result in more skillful ensemble forecasts.

181 A fundamental argument, that has been often overlooked, is that the merit of stochastic
182 parameterization goes far beyond providing uncertainty estimations for weather and climate
183 predictions, but may be also needed for better representing the mean state (e.g., Sardeshmukh et
184 al. 2001, Palmer 2001, Berner et al. 2008) and regime transitions (e.g., Williams et al. 2003,
185 2004, Birner and Williams 2008, Christensen et al. 2015a) via inherent non-linear processes.
186 This is especially relevant for climate projections, which have long-standing mean state errors,
187 such as e.g., a double inter-tropical convergence zone (e.g., Lin et al. 2007), and erroneous
188 stratocumulus cloud cover, which play a crucial role in the climate response to external forcing.

189 Mechanisms for how Gaussian zero-mean fluctuations can change the mean state (see Figure 1)
190 have been discussed e.g. in Tompkins and Berner (2008) and Beena and von Storch (2009).
191 Tompkins and Berner (2008) introduce perturbations to the humidity field and find that positive
192 perturbations are more likely to trigger a convective event than negative perturbations can
193 suppress convection. Beena and von Storch (2009) study the ocean response air-sea flux
194 perturbations and similarly find that negative buoyancy anomalies result in an altered
195 stratification, while positive anomalies tend to sustain the existing stratification. Insofar as
196 stochastic parameterizations can change the mean state, they have the potential to affect the
197 response to changes in the external forcing (e.g., Seiffert and von Storch 2008).

198 In mathematical terms, this is the question how a stochastic forcing affects the invariant measure
199 of a deterministic dynamical system (Lucarini 2012) and how the climate response to such a
200 forcing can be framed as a problem of non-equilibrium statistical mechanics (Colangeli et al.
201 2012, 2014, Lucarini and Sarno 2011, Lucarini et 2014a,b).

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

203 • Estimating uncertainty in weather and climate predictions

204 • Reducing systematic model errors arising from unrepresented subgrid-scale fluctuations

205 • Triggering noise-induced regime transitions

206 • Capturing the response to changes in the external forcing

207 and should be applied in a systematic and consistent fashion, not only to weather, but also to
208 climate simulations.

209 Several studies have identified the assessment of the benefits of stochastic closure schemes as
210 key outstanding challenge in the area of mathematics applied to the climate system (Palmer
211 2001, 2012, Palmer and Williams 2008, Williams et al. 2013). For accessible reviews of
212 rigorous mathematical approaches applied to weather and climate, we refer to Penland
213 (2003a,b), Majda et al. (2008) and Franzke et al. (2015). The current study focuses on recent
214 developments and successful applications of empirical and rigorous approaches to the subgrid-
215 parameterization problem in weather and climate models.

216 2 Representing Uncertainty in Comprehensive Climate and Weather Models

217 *2.1 Adding uncertainty a posteriori: the stochastically perturbed parameterization tendency*
218 *scheme and the stochastic kinetic-energy backscatter scheme*

219 Stochastic parameterizations are based on the notion that – as spatial resolution increases – the
220 method of averaging (Arnold 2001, Monahan and Culina 2011) is no longer valid and the
221 subgrid-scale variability should be sampled rather than represented by the equilibrium mean. In
222 addition, unrepresented interactions between unresolved subgrid-scale processes with the large-

scale flow might affect the resolved dynamics.

Former is addressed by the stochastically perturbed parameterization tendency (SPPT) scheme, which perturbs the net tendencies of the physical process parameterizations (convection, radiation, cloud physics, turbulence and gravity wave drag). One essential feature for its success 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, Teixeira and Reynolds 2008, Palmer et al. 2009, Weisheimer et al. 2014, Christensen et al. 2015b, Dawson and Palmer 2015, Batté and Doblas-Reyes 2015). SPPT tends to be most active in the tropics and near the surface, where the parameterized tendencies are large.

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. For this purpose, the scheme re-injects a small fraction of the dissipated energy into the resolved flow. Originally developed in the context of Large Eddy Simulations (LES; Mason and Thomson 1992), it was adapted by Shutts (2005) for Numerical Weather Prediction (NWP).

Depending on the details of the implementations, SKEBS tends to have most impact in the storm-track regions and in the free atmosphere above the boundary layer and permits the physical parameterization schemes to adjust to a slightly perturbed large-scale background flow. Its beneficial impact on weather and climate forecasts are reported e.g., in Berner et al. (2011, 2015), Tennant et al. (2011), Weisheimer et al. (2014), Sanchez et al. (2015); albeit Shutts (2013) criticizes the arbitrary nature of some of the design features based on coarse-graining high-resolution simulations to compute the backscatter term. His stochastic convective backscatter scheme (Shutts, 2015) includes a phase relationship between flow and perturbations

and adds additional perturbations to the divergent flow to remedy some of the identified shortcomings.

While these schemes are motivated by physical reasoning and scheme parameters are informed in some manner, for example by coarse-graining high-resolution output (Shutts and Palmer 2007, Shutts and Callado Pallarès 2014) or comparison with observations (Watson et al. 2015), the perturbations are essentially empirical constructs. For example, the amplitude of the perturbations is typically determined as the value that satisfactorily reduces the ensemble 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 the increase in spread. However, Berner et al. (2015) found that the merits of stochastic parameterization go beyond increasing spread and can account for structural model uncertainty.

In the following examples, we show recent results that demonstrate the potential of stochastic parameterizations to improve the mean state representation and variability as well as the skill of seasonal forecasts.

First, we present recent results from the seasonal forecasting system at ECMWF. In the simulations with both, SPPT and SKEBS, excessively strong convective activity over the Maritime Continent and the tropical Western Pacific is reduced, leading to smaller biases in outgoing longwave radiation (Figure 2, adapted from Weisheimer et al. 2014), cloud cover, precipitation and near-surface winds. The stochastic schemes also lead to an increase in the frequency (Figure 3, from Weisheimer et al. 2014) and amplitude of MJO events, which is

an improvement. A reduction of excessive amplitudes in westward propagating convectively coupled waves in an earlier model version is reported in Berner et al. 2012.

Another example of the positive impact of stochastic schemes is evident in climate simulations with the Community Earth System Model (CESM). Compared to observations, the modeled spectrum of average sea surface temperature in the Nino 3.4 region has three times more power for periods between 2 and 4 years (Figure 4, adapted from Christensen et al. 2016). SPPT markedly reduces the temperature variability in this frequency range, leading to a much better agreement with nature (Christensen et al., 2016). Interestingly, in these examples adding stochasticity results in *reduced* variability, which is a non-trivial response.

Along with the improvemed model climate, stochastic perturbations benefit probabilistic forecast performance on seasonal timescales. This has been reported in a number of studies using earlier versions of ECMWF's seasonal system (Berner at al. 2008, Dobles-Reyes et al. 2009, Palmer at al. 2009) and recently been confirmed in the newest version (Weisheimer et al. 2014) and in the EC-Earth system model (Batté and Doblas-Reyes 2015). Figure 5 shows ensemble mean and spread in forecasts for Nino 3.4 area sea-surface temperatures with the EC-Earth model, run at a standard horizontal resolution (SR, ca. 60km for the atmospheric and ca. 100km for the ocean component) and a high resolution (HR, ca. 40km for the atmospheric component and 25km for the ocean.) For both resolutions, the introduction of SPPT perturbations increases the ensemble spread. Furthermore, SPPT reduces the mean error in the standard resolution, but not as much as increasing horizontal resolution.

290 A number of studies have found evidence for stochasticity leading to noise-induced
291 transitions in mid-latitude circulation regimes, especially over the Pacific-North America
292 region (Jung et al. 2005, Berner et al. 2012, Dawson et al. 2015, Weisheimer et al. 2014).
293 These results suggest that stochastic parameterizations are also relevant for the prediction of
294 the dominant modes of atmospheric variability such as the North Atlantic Oscillation and
295 the Pacific North American pattern (Berner et al. 2016).

296 ***2.2 Adding uncertainty a priori: perturbed parameter approaches for the atmospheric***
297 ***component***

298 While the performance of the stochastic schemes discussed in the last section is undisputed,
299 they have been criticized in that they are added *a posteriori* to models that have been
300 independently developed and tuned. Ideally, stochastic perturbations should represent
301 model uncertainty where it occurs. One obvious way to represent uncertainty at its source
302 rather than *a posteriori* is the perturbed parameter approach, which perturbs the closure
303 parameters in the physical process parameterizations. There are two variants: the parameter
304 can be fixed throughout the integration, but vary for each ensemble member (e.g. Murphy
305 et al. 2004, Hacker et al. 2011a) or vary randomly with time (e.g. Bowler et al. 2008, 2009,
306 Ollinaho et al. 2013, Jankov et al., 2016). Strictly, the first variant is not a stochastic
307 parameterization, but an example for a multi-model, since each ensemble member has a
308 different climatology. However, since stochastic parameter perturbations are routinely
309 compared to fixed-parameter schemes, this section discusses both.

310 While perturbed-parameter ensembles typically outperform unperturbed ensembles on
311 weather timescales, they typically cannot sufficiently account for all deficiencies in the
312 spread (Hacker et al. 2011, Reynolds et al. 2011, Christensen et al. 2015b) and do not lead

313 to the same reliability as the *a posteriori* schemes discussed above (Berner et al., 2015).
314 Presumably, this is due to the fact that *a posteriori* schemes are designed to
315 encapsulate all model uncertainty, of which parameter uncertainty is only one
316 contributor.

317 An ensemble system is considered statistically reliable when a predicted probability for a
318 particular event (e.g. temperature exceeding 17°C) compares well with the observed
319 frequencies. Another limitation of this approach is that the parameter uncertainty estimates
320 are subjective, and information about parameter interdependencies is not included.

321 The following studies are examples for applications of the perturbed-parameter approach to
322 physical process parameterizations and perturbing the interface between different model
323 components. We start with results pertaining to perturbations in the atmospheric
324 component and move to those of other model components, such as land and ocean models,
325 which are more relevant for climate applications.

326 A number of studies report on improved skill due to parameter perturbations to boundary
327 layer and convection schemes (Hacker et al. 2011, Reynolds et al. 2011, Jankov et al.,
328 2016). Recently, a stochastic "eddy-diffusivity/ mass-flux" parameterization has been
329 developed (Suselj et al. 2014), which combines an eddy-diffusivity component with a
330 stochastic mass-flux scheme. The resulting scheme unifies boundary layer and shallow
331 convection and was operationally implemented in the operational Navy Global
332 Environmental Model.

333 Christensen et al. (2015b) used an objective covariance estimate of parameter uncertainty
334 (Järvinen et al. 2012, Ollinaho et al. 2013) for four convection closure parameters and developed

335 both a fixed-parameter and a stochastically varying perturbation scheme. Both schemes
336 improved the forecast skill of the ECMWF ensemble prediction system, with a larger impact
337 observed for the fixed perturbed parameter scheme (Figure 6, adapted from Christensen et al.
338 2015b). In addition, for some variables such as wind at 850hPa, the scheme leads to a reduction
339 in bias (Figure 6, adapted from Christensen et al. 2015b).

340 Recently, a body of work proposes stochastic approaches for another atmospheric
341 parameterization, namely non-orographic gravity waves (Lott et al. 2012, Lott and Guez 2013,
342 and de la Cámara and Lott 2015). Observational studies indicate that the gravity wave field is
343 very intermittent and only predictable in a statistical sense. Recently, de la Cámara et al. (2014)
344 informed the free parameters of the stochastic gravity-wave scheme using momentum flux
345 measurements.

346 ***2.3 Uncertainty in land surface, ocean and coupled component models***

347 Physical parameters of land surface models are often not well constrained by observations. A
348 recent study by MacLeod et al. (2015) introduced parameter perturbations to key soil
349 parameters, and compared their impact with stochastic perturbations of the soil moisture
350 tendencies in seasonal forecasts with the ECMWF coupled model. Both the perturbed parameter
351 approach and the stochastic tendency perturbations improved the forecasts of extreme air
352 temperature for the European heat wave of 2003.

353 A shortcoming in land models stems from the omission of sub-grid land heterogeneity, which
354 impacts the surface heat flux. Langan et al. (2014) retained the subgrid-variability by drawing
355 the area for each plant functional types at each timestep from a Dirichlet distribution, rather than
356 using constant area weights. First results with a single column model version of CESM reveal an
357 increase in the variability as well as larger extreme values in convective precipitation (Figure 7,

358 adapted from by Langan et al. 2014).

359 The coupled atmosphere-ocean system is very sensitive to fluctuations in the fluxes between its
360 component models. Air-sea fluxes of buoyancy, energy, and momentum vary on a vast range of
361 space and time scales, including scales that are too small or fast to be explicitly resolved by
362 global climate models. For example, convective clouds in the atmosphere will cause subgrid
363 fluctuations at the air-sea interface, in both, the downward fresh water flux and short-wave solar
364 radiation. The response of the climate to stochastic perturbations of the air-sea buoyancy flux is
365 studied by Williams (2012) in a coupled atmosphere-ocean model. The response is complex and
366 involves changes to the oceanic mixed-layer depth, sea-surface temperature, atmospheric Hadley
367 circulation, and fresh water flux across the sea surface (Figure 8, from Williams 2012). These
368 findings suggest that the lack of representation of stochastic subgrid variability in air-sea fluxes
369 may contribute to some of the biases exhibited by contemporary coupled climate models.

370 Since the buoyancy effects in the ocean are different from that in the atmosphere, the length
371 scale at which rotational effects become as important as gravity wave effects is much smaller.
372 Consequently, mesoscale eddies in state-of-the art ocean models are still far from being resolved
373 and are usually represented by traditional bulk parameterizations (Gent and McWilliams 1990,
374 Redi 1982). A recent study by Li and von Storch (2013) computes the contributions from the
375 mean and fluctuating component of heat flux divergence in a high-resolution ocean model. The
376 magnitude of the fluctuations is about one order of magnitude larger than the mean component
377 (Figure 9, adapted from Li and von Storch 2013) suggesting that classical parameterizations
378 significantly underestimate the total eddy flux. The fluctuating part, even though having zero
379 mean, can play an important role in generating large-scale low-frequency variations and in
380 shaping the mean oceanic circulation.

Juricke et al. (2013) and Juricke and Jung (2014) recently investigated the sensitivity of an ocean-sea ice model to variations in the ice strength parameter. As this parameter is not observable, large uncertainties remain in the choice of its value, although it is very important for modeling sea ice drift. Varying this parameter stochastically results in changes to the mean sea ice distribution as well as sea ice spread. Compared to perturbations of the atmospheric initial conditions, the incorporation of additional stochastic ice strength perturbations leads to a considerably increase in spread of the simulated sea ice thickness in the central Arctic (Figure 10, adapted from Juricke et al. 2014), which is a better match with the observed uncertainties (Juricke et al. 2014).

2.4 Data Assimilation and Extreme Events

The purpose of data assimilation is to combine observations with short-term model-forecasts to come up with a gridded and physically consistent estimate of the state of the atmosphere, also called "analysis". One method is to use short-term forecasts as the first guess fields in ensemble data assimilation. As such, ensemble data assimilation inherits the shortcomings of short-term ensemble predictions, namely, the underdispersivness in the spread. Recent work has demonstrated that the stochastic parameterizations that are beneficial for ensemble prediction, can also improve analyses fields (Isaksen et al. 2007, Houtekamer et al. 2009, Mitchell and Gottwald 2012, Hamill and Whitaker 2011, Ha et al. 2015, Romine at al. 2015). In particular, Ha et al. 2015 showed that the inclusion of a stochastic parameterization improved the mean analysis, even if the observations were constrained to those in the control experiment. A cutting-edge frontier is the use of memory effects in Kalman filter data assimilation schemes (O'Kane and Frederiksen 2012).

The impact of stochastic perturbations on extremes has only been considered very recently. A

404 body of work focuses on the description of non-Gaussian subgrid-scale processes (Majda et al.
405 2009, Sardeshmukh and Sura 2009, Sura 2011, Sardeshmukh et al. 2015). Franzke (2012)
406 showed that his reduced stochastic model (see next section) captures the extremes of the full
407 model. He et al. (2012) studied the influence of an explicitly stochastic representation of mixing
408 in the stable boundary layer on the extremes of near-surface wind speed in a single column
409 model. Tagle et al. (2015) were the first to study the effect of the stochastic parameterizations in
410 a comprehensive climate model. They found that the stochastic parameterizations had a big
411 impact on the surface temperature mean and variability, but hardly changed the tail behavior.

412 # 3 Systematic mathematical and statistical physics approaches

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

416 ## *3.1. Mathematical and Numerical implications of stochasticity*

417 Although the motions of the atmosphere and ocean are described by the Navier-Stokes
418 equation, large-scale flows can often be modeled under hydrostatic approximation. This
419 leads to the deterministic primitive equation system. If we want to represent continuous
420 small-scale fluctuations as stochastic terms, these equations need to be generalized to allow
421 for stochasticity. A relevant mathematical field is thus the extension of the derivation to the
422 stochastic primitive equations for two-dimensional (Ewald et al. 2007; Glatt-Holtz and
423 Ziane 2008; Glatt-Holtz and Temam 2011) and three-dimensional flows (Debussche et al.
424 2012).

425 Moreover, stochastic systems require calculi and numerical schemes fundamentally
426 different from the ones available to solve deterministic systems. The two most commonly
427 used stochastic integral types are the Itô-integral (Itô 1951) and the Stratonovich-integral
428 (Stratonovich 1966). When the fast processes of a continuous system are modeled by white
429 noise – as is common for physical applications - the resulting stochastic model converges to
430 a Stratonovitch stochastic differential equation (Wong and Zakai 1965, Papanicolaou and
431 Kohler 1974, Gardiner 1985, Penland 2003a,b). Discrete systems converge to the Itô
432 stochastic differential equation. Starting in the 1970s a solid framework of numerical
433 methods for stochastic ordinary differential equations was developed (Rümelin 1982,
434 Kloeden and Platen 1992, Milstein 1995, Kloeden 2002). However, this has been extended
435 to high-order schemes only recently (Jentzen and Kloeden 2009, Weniger 2014). With
436 stochastic parameterizations becoming more common in weather and climate simulations, a
437 revision of the deterministic numerical schemes should be undertaken to ensure the
438 convergence of the numerical solutions.

439 ***3.2 Homogenization and stochastic mode reduction***

440 Numerical weather and climate modeling can be seen as a model reduction problem. Because
441 we cannot numerically solve the full continuous equations, we have to truncate the equations at
442 some scale and then treat the unresolved processes in some smart way. A systematic approach
443 for the derivation of reduced order models from first principles is performed through the method
444 of homogenization or adiabatic elimination (Wong and Zakai 1965, Khas'minskii 1966, Kurtz
445 1973, Papanicolaou and Kohler 1974, Pavliotis and Stuart 2008). The fundamental idea is to
446 decompose the state vector into slow and fast components, represent the fast processes by a
447 stochastic term and derive analytically an effective equation for the slow, predictable modes.

448 Majda et al. (1999) and Majda et al., 2001 expanded this body of work by making additional
449 assumptions on the nonlinear self-interaction of the fast modes and coined the term "stochastic
450 mode reduction".

451 The stochastic mode reduction has been demonstrated to successfully model regime-behavior
452 and low-frequency variability for conceptual models of the atmosphere (Majda et al. 2003), the
453 barotropic vorticity (Franzke et al. 2005) and a quasi-geostrophic three-layer model on the
454 sphere with realistic orography (Franzke and Majda 2006). However, due to both, the sheer
455 amount of analytical derivation and the compute-memory requirement in the numerical
456 implementation of the resulting equations, the stochastic mode reduction cannot be easily
457 applied to comprehensive climate models of arbitrary complexity. A possible way forward is to
458 apply the stochastic mode reduction locally at each gridpoint rather than globally (Dolaptchiev
459 et al. (2013 a,b).

460 These mathematical techniques are rigorously valid only in the limit of large time-scale
461 separation, although some studies report good empirical results, even when this condition is not,
462 or only partly met (Dozier and Tappert 1978a,b , Majda et al. 2003 2008, Franzke et al. 2005,
463 Franzke and Majda 2006). When the time scale separation between the fast and slow processes
464 is not too large, the picture of the parameterization as being constructed as the sum of a suitably
465 defined deterministic plus random corrections has to be amended to take memory effects into
466 account (e.g. Zwanzig 2001, Chekroun et al. 2015a,b). Unfortunately, the condition of scale
467 separation is typically not met in geophysical fluid dynamics applications (Sardeshmukh and
468 Penland 2015, Yano 2015, Yano et al. 2015), which poses limitations to the application of
469 homogenization. An alternative, which does not make any assumptions about time scale
470 separation and provides an explicit expression for the terms responsible for the memory effect is

proposed by Wouters and Lucarini (2012, 2013), who, instead, assume the presence of a weak dynamical coupling between the fast and the slow scales of motion.

The question of which stochastic process is best suited to describe the nonlinear interactions of the unresolved processes is an open topic. While methods for Gaussian diffusion processes are well known (Oppenheim 1975) it may be the case that other formulations like Lévy processes are better suited to describe the underlying physics. For the interested reader, we refer to recent studies by 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 Physics to Weather and Climate

The scale-aware representation of convection and clouds on high-resolution grids (1-50 km) has been a long-standing challenge for weather and climate models. Within a single model column, convection is not uniquely determined by the resolved-scale processes, and the distribution of possible realizations of subgrid-scale convection highly depends on model resolution. Furthermore, horizontal transports of heat, moisture or momentum from neighboring grid-boxes are typically neglected. Thus, to achieve scale-awareness, it is necessary to represent scale-dependent convective fluctuations about the ensemble average response. In addition, because of the lack of time-scale separation, a correct representation of convection across scales requires memory of subgrid-states from previous time steps.

A novel approach to represent the fluctuations in an ensemble of deep convective clouds adapts concepts from statistical mechanics (Craig and Cohen 2006). Based on this theory, a stochastic parameterization of deep convection was developed to represent fluctuations of the subgrid

493 convective mass flux about statistical equilibrium (Plant and Craig 2008). This is especially
494 attractive for variable-resolution grids, since the statistics automatically adapt to the grid-
495 resolution. This approach was extended to shallow convective clouds by introducing a memory
496 effect arising from the correlation between the cloud mass fluxes and cloud lifetimes (Sakradzija
497 et al. 2015). Figure 11 (adapted from Sakradzija et al. 2015) shows histograms of the subgrid
498 cloud-base mass flux in the stochastic shallow cumulus cloud scheme and coarse-grained large-
499 eddy simulation at different horizontal resolutions. The histograms match closely and are scale-
500 aware.

501 ***3.4 Modeling convective processes by Markov chains and cellular automata***

502 Another way to introduce temporal memory and nonlocal effects is the use of Markov
503 chains and cellular automata. A Markov chain is a mathematical system that undergoes
504 transitions from one *discrete* state to another and the probabilities associated with the
505 various state changes are called transition probabilities. If observational data or high-
506 resolutions simulations are used to inform the transition probabilities, the Markov chains
507 are called data-driven.

508 An example for this approach is the "stochastic convective parameterization" which
509 describes the convective state of the entire model column as a discrete Markov chain.
510 (Khouider et al. 2010, Dorrestijn et al. 2013a,b, 2015, Gottwald et al. 2015). The system
511 can only reside in a few distinct convective states – e.g., but not necessarily: clear sky,
512 shallow or deep convection, - and the random transitions from one state to another evolve
513 as a Markov chain. For example, Dorrestijn et al. 2013a cover the horizontal domain of the
514 numerical model with a high-resolution lattice (with typical lattice spacing of 100m to
515 1000m), and on each lattice node lives a copy of the discrete stochastic process for the

convective state (Figure 12, adapted from Dorrestijn et al. 2013a). The transition probabilities are estimated from a cloud-resolving LES model. By averaging over blocks of lattice nodes, convective area fractions and related quantities can be obtained for spatial domains of arbitrary size. The resulting patterns and temporal behavior of the area fractions are 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 is scale-adaptive.

Frenkel et al. (2012) and Peters et al. (2013) use the stochastic model introduced in Khouider et al. (2010), but different methods to estimate the transition probabilities. Khouider et al (2010) and Frenkel et al. (2012) formulate the rules based on physical insight, while Peters et al. (2013) use observations for their estimates. Latter find that the estimates from observation can notably differ from those based on physical intuition.

A related approach are cellular automata which are often used as simple mathematical models to simulate spatial self-organizational behavior such as convective organization A cellular automaton describes the evolution of discrete states on a lattice grid. The states are updated according to a set of rules based on the states of neighboring cells at the previous time step. In addition to memory, cellular automata can allow for lateral communications between neighboring grid boxes and thus introduce spatial correlations.

The idea of using cellular automata within NWP was first proposed by Palmer (2001) and first applications used them as a quasi-stochastic pattern generator for SKEBS (Shutts 2005, Berner et al. 2008). Bengtsson et al. (2013) pioneered the use of a cellular automaton for the parameterization of convection, which allows for the horizontal transports of heat, moisture and momentum across neighboring grid-boxes. The scheme has been shown to

539 enhance the organization of convective squall-lines (Bengtsson et al. 2013) and improves
540 the skill of accumulated precipitation in a high-resolution ensemble prediction system
541 (Bengtsson and Körnich 2015).

542 ***3.5 Climate Response in the presence of small-scale fluctuations***

543 While there is extensive work focusing on the response of the climate system to changes in
544 the external forcing, either natural - such as the forcing from a localized tropical heating as
545 it occurs in Nino - or anthropogenic - such from increased greenhouse gases, little attention
546 has been given to the fact if and how the representation of the subgrid-scale can alter that
547 response. In the mathematical community, this is the topic of response theory and the
548 fluctuation-dissipation theorem (e.g., Marconi et al. 2008, Lacorata and Vulpiani 2007,
549 Colangeli et al. 2011, Lucarini and Colangeli 2012, Colangeli and Lucarini 2014).

550 Seiffert and von Storch (2008) were the first to investigate the response of a climate model
551 to CO2-forcing in the presence of subgrid-scale fluctuations in atmospheric temperature,
552 divergence and vorticity. In their model, the strength of the global warming due to a CO2-
553 doubling is altered by up to 15% near the surface and up to 25% in the upper troposphere
554 (Figure 13, from Seiffert and von Storch 2008) depending on the exact representation of the
555 small-scale fluctuations. Applying a stochastic model to their simulations, they found that
556 the small-scale fluctuations change the temperature response via a statistical damping
557 that acts as a restoring force. In addition, the small-scale fluctuations can affect feedback
558 and interaction processes that are directly coupled to an increase in CO2, thereby altering
559 the CO2-related radiative forcing (Seiffert and von Storch 2010).

560 The fluctuation-dissipation theorem (FDT) is concerned with the response of a system to
561 small changes in the forcing. In particular, it tries to relate the response to the natural

562 fluctuations in the system (Kubo 1966, Deker and Haake 1975, Hänggi and Thomas 1977,
563 Leith 1975, Risken 1984). In the atmospheric sciences, the FDT-operator is estimated from
564 model output, in particular the variances and covariances of the state variables at different
565 time lags. The so obtained empirical linear model is able to predict the response to changes
566 in the external forcing, such as signature from localized tropical heat forcing (Gritsun and
567 Branstator 2007, Gritsun et al. 2008).

568 Achatz et al. (2013) argue that subgrid-scale parameterizations developed for a present day
569 climate, might no longer be accurate in a changing climate. They use the FDT to adjust the
570 subgrid-scale representation of the forced system. Figure 14 (adapted from Achatz et al.
571 2013) shows that a low-order model with a subgrid-scale parameterization corrected by the
572 FDT yields a better response in streamfunction variance than without the correction.

573 While some success of FDT-techniques to low-frequency climate modeling has been
574 demonstrated, some of the mathematical assumptions are not strictly met. Recent work expands
575 the mathematical underpinning by formulating the response theory more generally and is better
576 suited for non-equilibrium systems (Ruelle 2009, Lucarini and Sarno 2011) and climate
577 projections (Lucarini et al. 2014, Ragone et al. 2015).

578 ***3.6 Statistical Dynamical Closure Theory***

579 Kraichnan (1959) first illustrated that renormalization of the statistical equations of fluid
580 motion can been used to produce self-consistent parameterizations of the subgrid turbulent
581 processes. It is on this basis that Frederiksen and Davies (1997) developed stochastic
582 parameterisations of subgrid turbulence in barotropic atmospheric simulations on the
583 sphere. The subgrid parameterizations consist of drain, backscatter and net eddy viscosities,
584 which are determined from the statistics of higher resolution closure simulations. The aim

585 here is that the spectra from the low-resolution simulation with stochastic subgrid
586 parameterization should be ideally statistically indistinguishable from those produced by
587 the high-resolution simulation, which would allow to save computational resources.
588 Implementation of this approach into an atmospheric GCM resulted in significantly
589 improved circulation and energy spectra (Frederiksen et al. 2003). These ideas were further
590 developed by Frederiksen (1999, 2012a,b), and O'Kane and Frederiksen (2008).

591 Frederiksen and Kepert (2006) then used the functional form of these closure approaches to
592 develop a zero-parameter stochastic modeling framework, where the eddy viscosities are
593 determined from higher-resolution reference simulations. This approach was successfully
594 applied to baroclinic geophysical simulations in Zidikheri and Frederiksen (2009, 2010a,b).
595 Recently, Kitsios et al. (2012, 2013,2014) used this approach to determine the eddy
596 viscosities from a series of high-resolution atmospheric and oceanic reference simulations.
597 The isotropized versions of the subgrid-eddy viscosities were then characterized by a set of
598 scaling laws. Large eddy simulations with subgrid models defined by these scaling laws
599 (solid lines in Figure 15) were able to reproduce the statistics of the high-resolution
600 reference simulations (dashed lines in Figure 15) across all resolved scales. This
601 demonstrates that including a stochastic subgrid parameterization in the low-resolution
602 simulations makes them indistinguishable from the high-resolution reference.
603 The scaling laws further enable the subgrid parameterizations to be utilized more widely, as
604 they remove the need to generate the subgrid coefficients from a reference simulation.

605 Concluding Remarks

606 In this article, we attempt to narrow the gap between the fields of numerical meteorological
607 models and applied mathematics in the development of stochastic parameterizations: on the one

608 hand geo-scientists are often unaware of mathematically rigorous results that can aid in the
609 development of physically relevant parameterizations, on the other hand mathematicians often
610 do not know about open issues in scientific applications that might be mathematically tractable.

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

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

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. 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. This is especially relevant for developing scale-aware parameterizations, where it is difficult to control the time scale separation as the spatial resolution is altered.

Of course, the stochastic approach is not a panacea for the subgrid-scale parameterization problem and persistent model biases. Stochastic approaches must complement developments in the deterministic physical process parameterizations and dynamical core, as motivated e.g. by Stevens and Bony (2013) and Jakob (2014). Nevertheless, it is our conviction, that basing stochastic parameterizations on sound mathematical and statistical physics 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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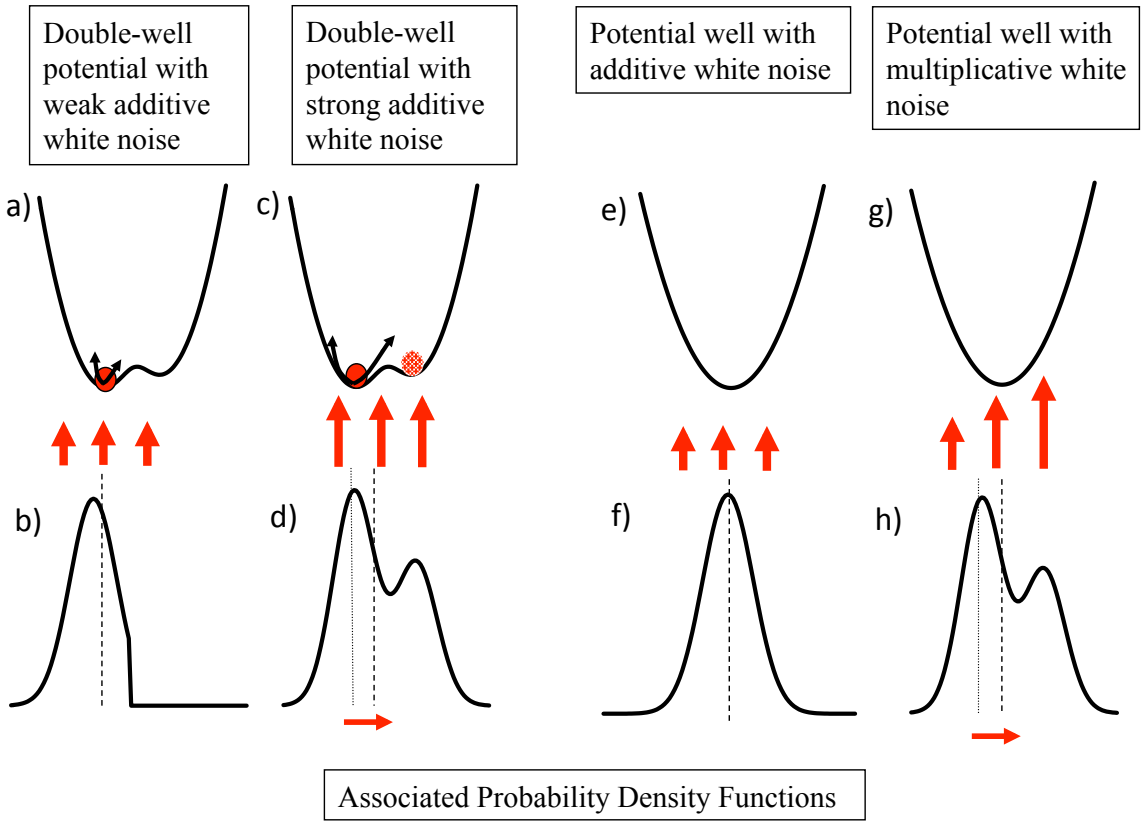

Figure 1: System characterized by a,c) double-potential or e,g) single-potential well and their associated probability density functions (PDFs). If the noise is sufficiently small (a) and under appropriate initial conditions, the system will stay in the deeper potential well and the associated probability 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 noise-induced changes the single-well potential of the unforced system, so that the effective potential including the effects of the multiplicative noise has multiple wells and the associated PDF becomes bimodal (h).

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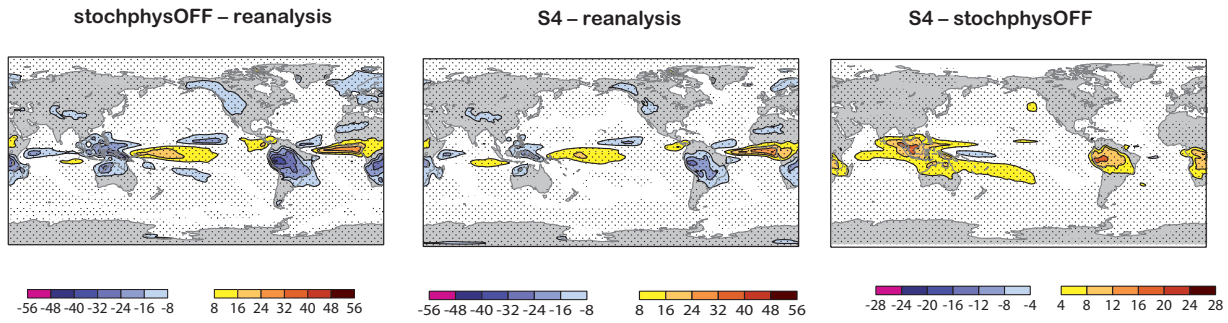

Figure 2: Bias in the top of the atmosphere net longwave radiation (outgoing longwave radiation) in W m–2 in DJF for the period 1981-2010. Simulations are conducted with ECMWF's seasonal forecasting System 4 with (S4) and without (*stochphysOFF)* stochastic parameterizations. Left and middle panels show difference from ERA-Interim reanalysis, right panel difference between experiments. Significant differences at the 95% confidence level based on a two-sided *t*-test are hatched. Adapted from Weisheimer et al. (2014).

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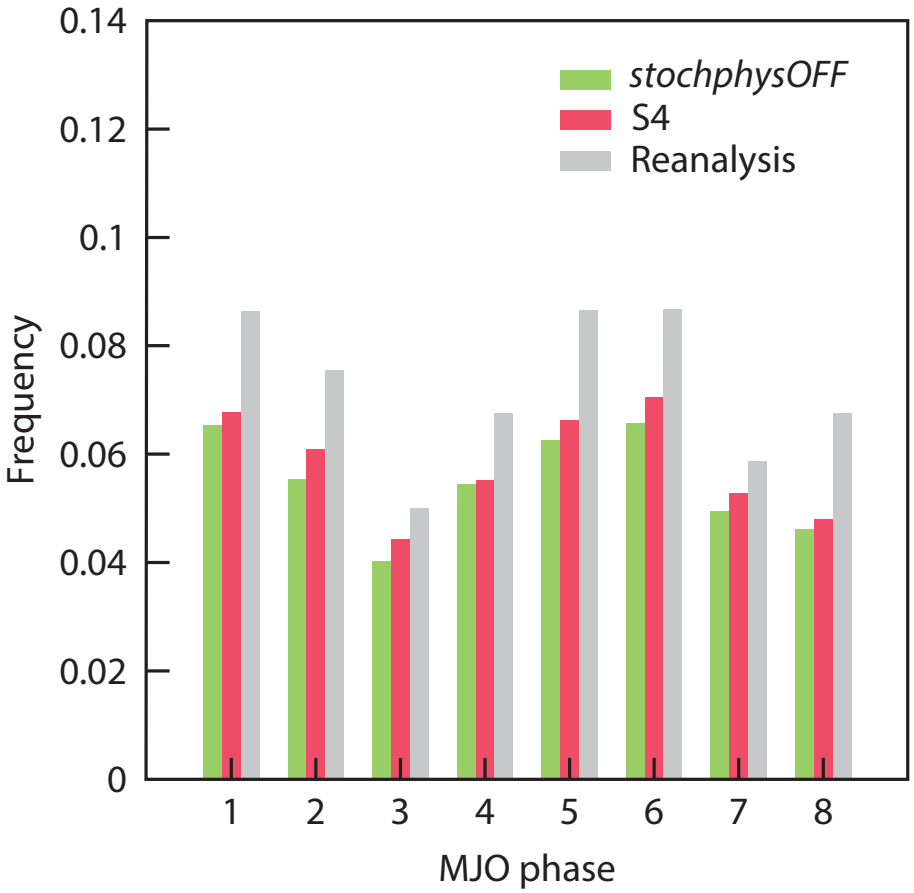

Figure 3: Relative frequencies of MJO events in each of the eight MJO phases for the period 1981-2010. Simulations are conducted with ECMWF's seasonal forecasting System 4 with (red) and without (green) stochastic parameterizations. Relative frequencies in ERA-Interim reanalysis in are shown in grey. From Weisheimer et al. (2014).

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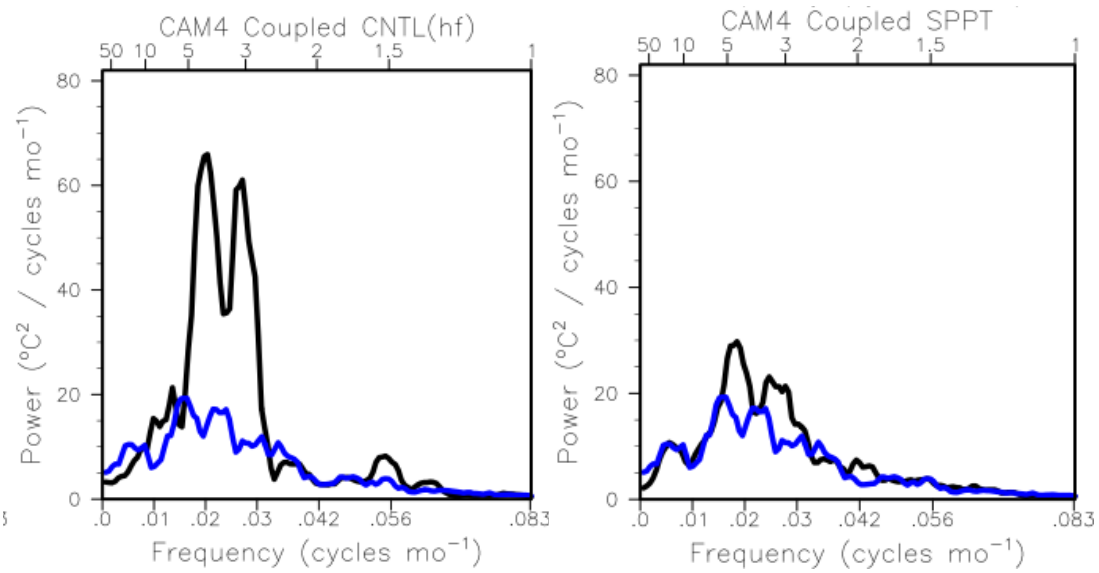

Figure 4: Power spectra of average sea surface temperature in the Nino 3.4 region in 135 year long simulations with the Community Earth System Model. Compared to HadISST observations (blue), the simulation has three times more power for oscillations with periods between 2 to 4 years (left). When the 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). Adapted from Christensen et al. (2016)©American Meteorological Society. Used with permission.

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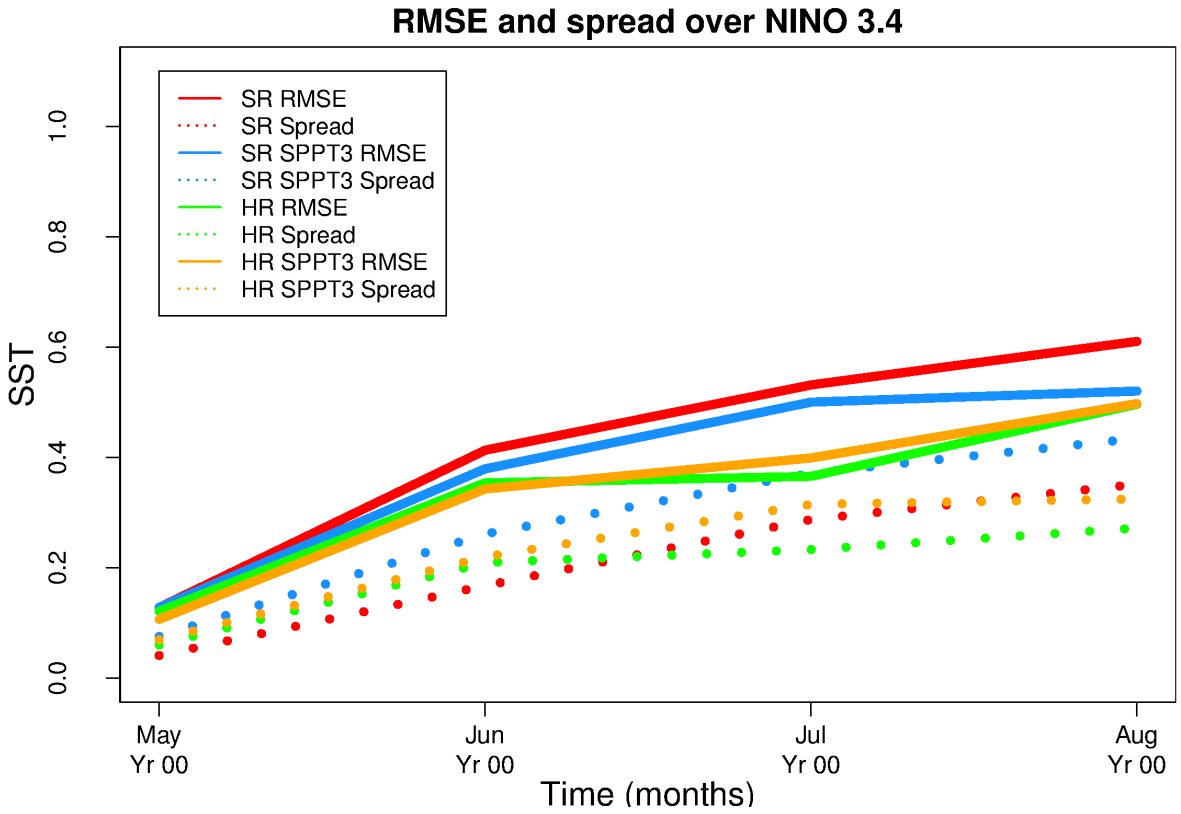

Figure 5: Niño 3.4 SST root mean square error (lines) and ensemble spread (dots) according to forecast time in EC-Earth 3 seasonal re-forecast experiments initialized in May 1993-2009 with standard (SR) or high resolution (HR) atmosphere and ocean components, with and without activating a 3-scale SPPT perturbation (SPPT3) method in the atmosphere.

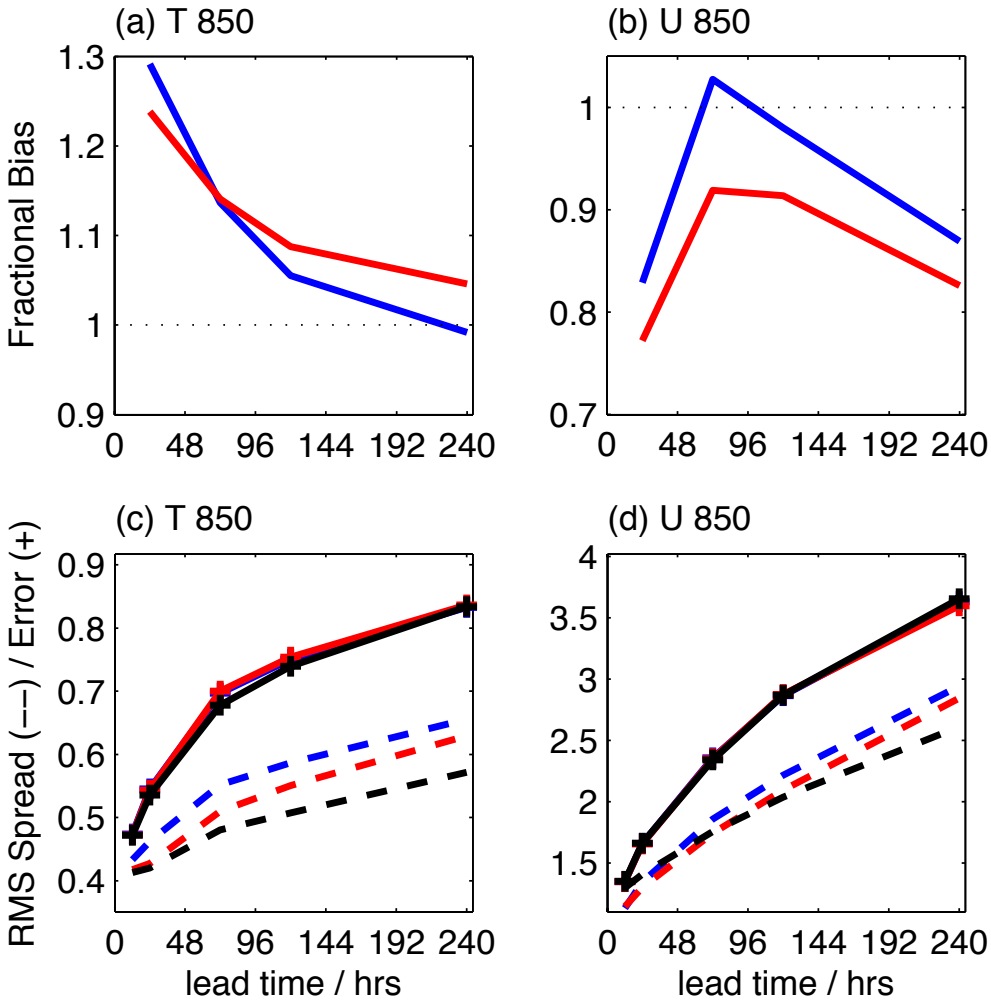

Figure 6: Forecast diagnostics as a function of time for the operational ECMWF IFS (black), fixed perturbed parameter (blue) and stochastically varying perturbed parameter (red) ensemble forecasts. Top: Forecast bias for (a) T850 and (b) U850 shown as a fraction of the bias for the operational system: 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. Adapted from Christensen et al. (2015b)©American Meteorological Society. Used with permission.

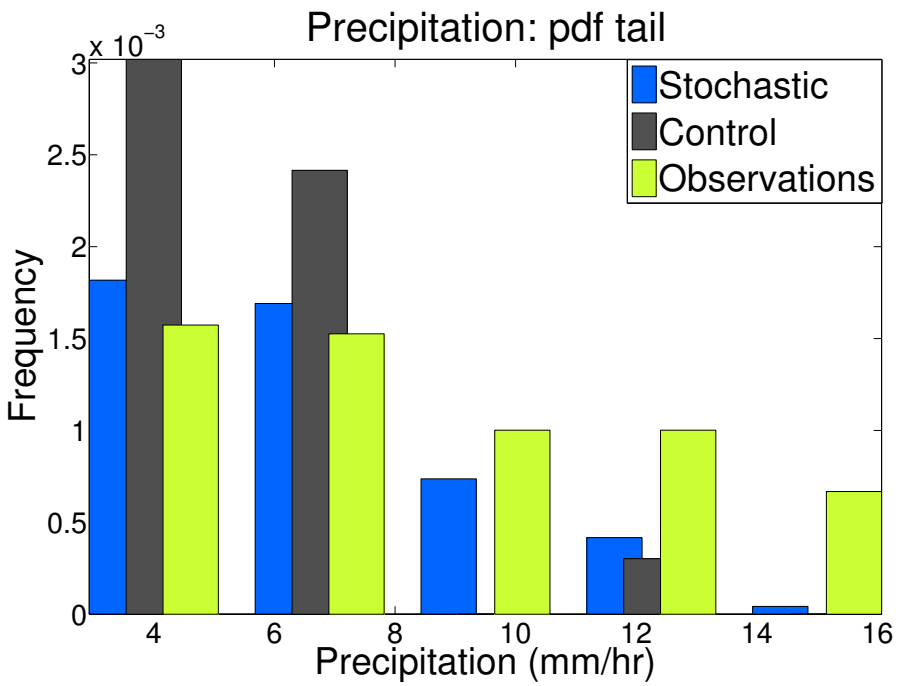

Figure 7: The right tail of the probability density function of summer season hourly precipitation from a 50-member ensemble of one year single column model simulations with stochastic (blue) and conventional parameterizations (black) of land cover over a model grid box encompassing the US Department of Energy's Atmospheric Radiation Measurement program's site in Lamont, Oklahoma. Observations are shown in green. 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°. Adapted from Langan et al. (2014) ©Elsevier. Used with permission.

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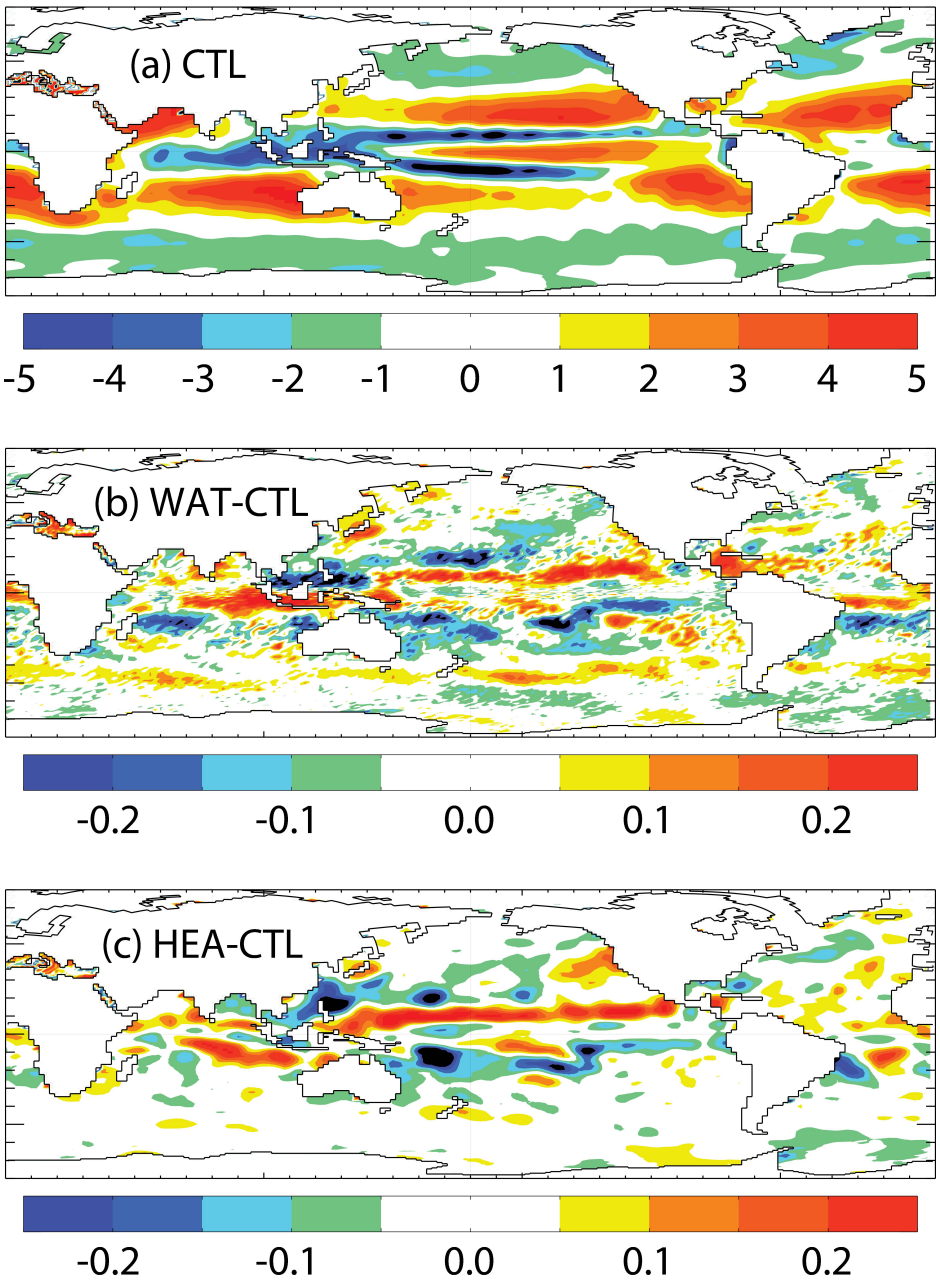

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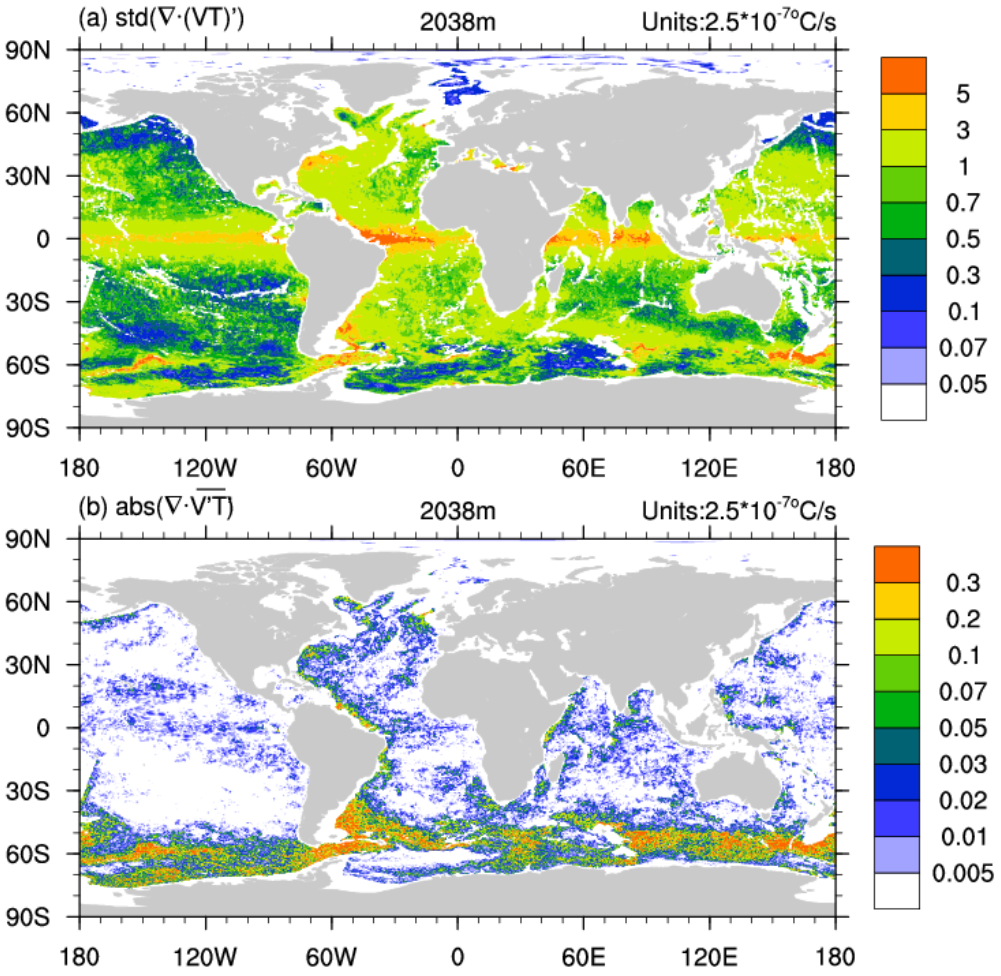

Figure 9: Top: Amplitude of fluctuations of the eddy forcing as measured by the standard deviation of divergence of eddy flux in a 1/10 degree OGCM. Bottom: Mean eddy forcing measured by the magnitude of the mean divergence of eddy heat flux in the same OGCM. The amplitude of the fluctuations is about one order of magnitude larger than the mean eddy forcing. Adapted from Li and von Storch (2013)©American Meteorological Society. Used with permission.

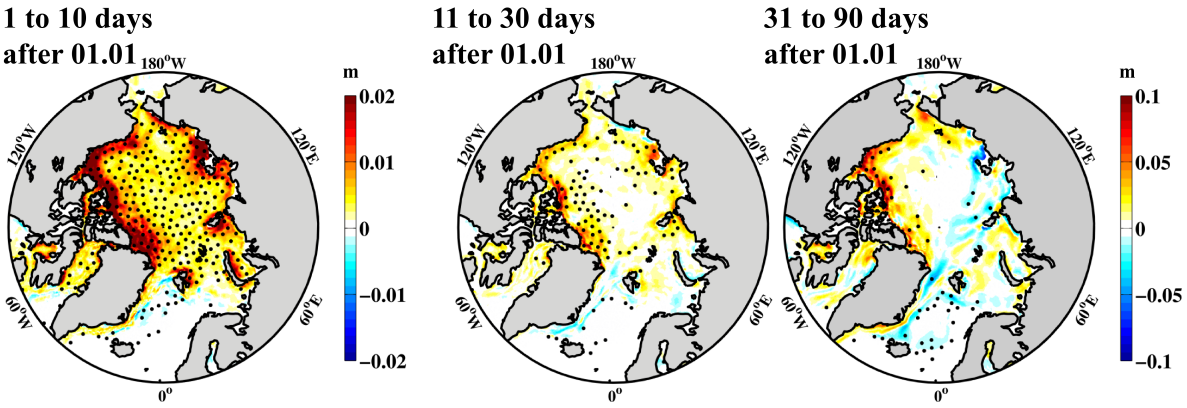

Figure 10: Difference in mean standard deviation of sea ice thickness forecasts (meters) between ensembles generated by stochastic ice strength as well as atmospheric initial perturbations and ensembles generated solely by atmospheric initial perturbations, averaged for days (left) 1 to 10, (middle) 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. Adapted from Juricke et al. (2014)©American Geophysical Union. Used with permission.

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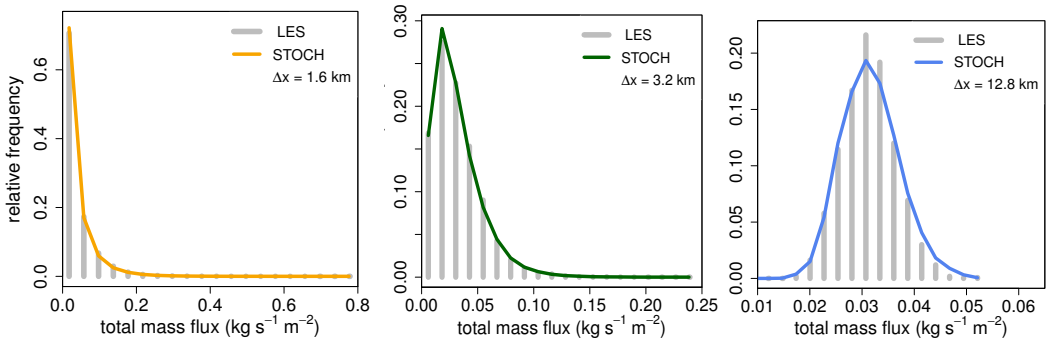

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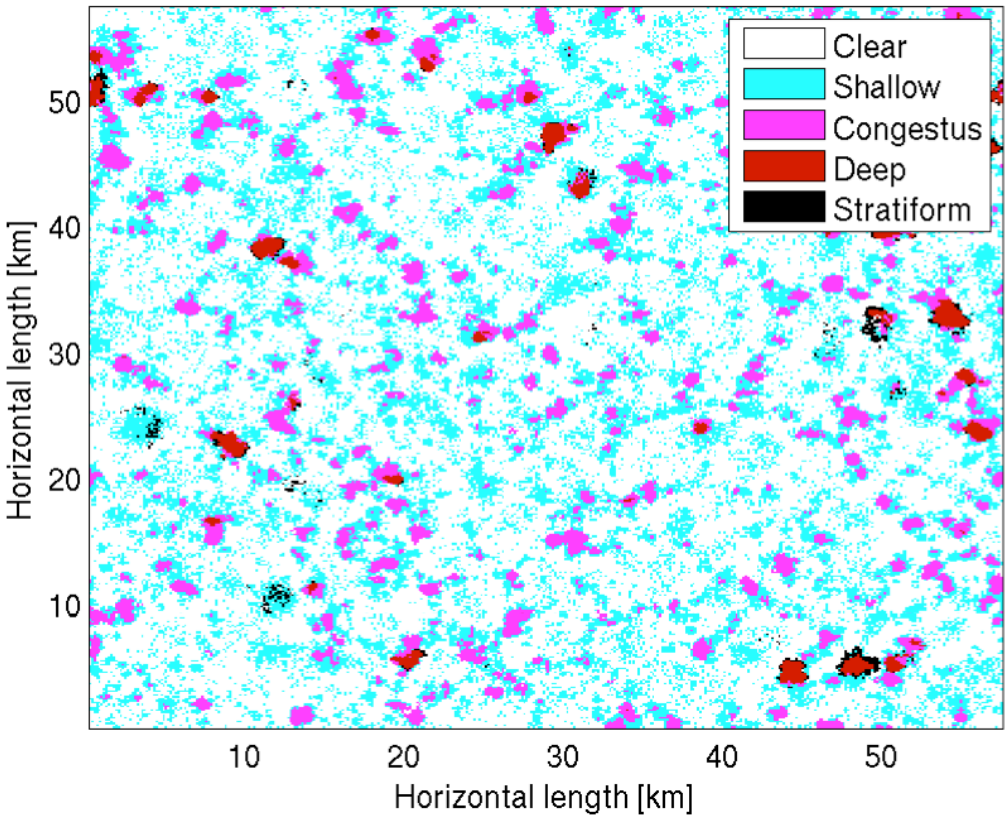

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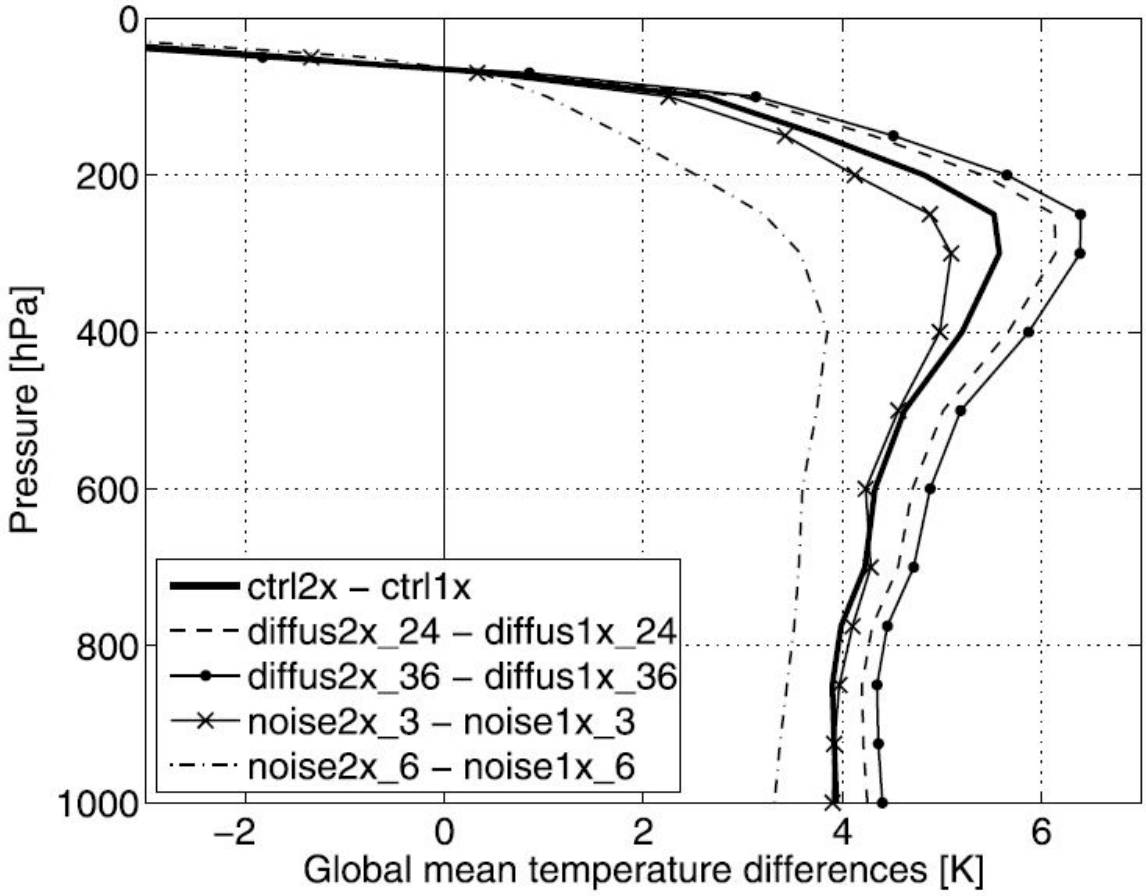

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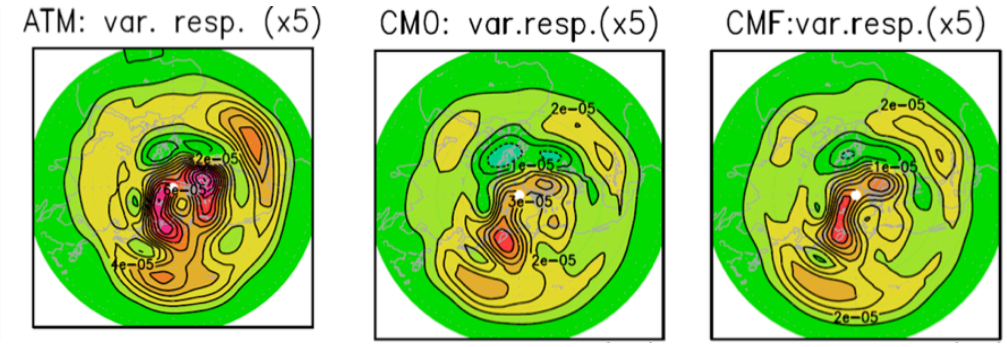

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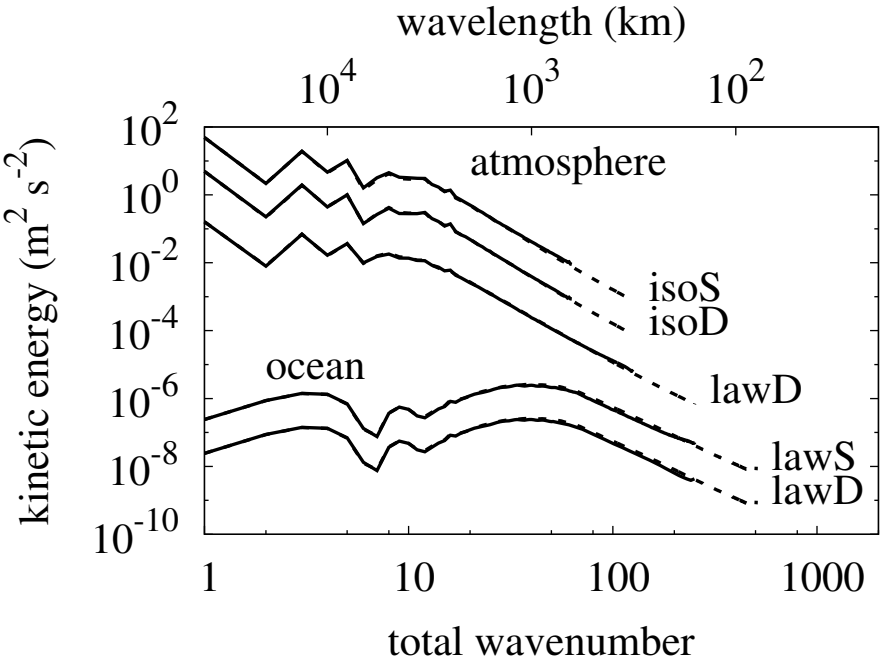

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