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

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65

66   **ABSTRACT**

67   The last decade has seen the success of stochastic parameterizations in short-term, medium-

68   range and seasonal forecasts: operational weather centers now routinely use stochastic

69   parameterization schemes to better represent model inadequacy and improve the quantification

70   of forecast uncertainty. Developed initially for numerical weather prediction, the inclusion of

71   stochastic parameterizations not only provides better estimates of uncertainty, but it is also

72   extremely promising for reducing longstanding climate biases and is relevant for determining

73   the climate response to forcing such as an increase of CO_2.

74   This article highlights recent developments from different research groups which show that the

75   stochastic representation of unresolved processes in the atmosphere, oceans, land surface and

76   cryosphere of comprehensive weather and climate models (a) gives rise to more reliable

77   probabilistic forecasts of weather and climate and (b) reduces systematic model bias.

78   We make a case that the use of mathematically stringent methods for the derivation of stochastic

79   dynamic equations will lead to substantial improvements in our ability to accurately simulate

80   weather and climate at all scales. Recent work in mathematics, statistical mechanics and

81   turbulence is reviewed, its relevance for the climate problem demonstrated, and future research

82   directions outlined.

83

84 **CAPSULE** (20-30 words)

85 Stochastic parameterizations - empirically derived, or based on rigorous mathematical and

86 statistical concepts - have great potential to increase the predictive capability of next generation

87 weather and climate models.

88

1 The need for stochastic parameterizations

89

90 Numerical weather and climate modeling is based on the discretization of the continuous

91 equations of motion. Such models can be characterized in terms of their dynamical core, which

92 describes the resolved scales of motion, and the physical parameterizations, which provide

93 estimates of the grid-scale effect of processes, that cannot be resolved. This general approach

94 has been hugely successful in that skillful predictions of weather and climate are now routinely

95 made (e.g. Bauer et al. 2015). However, it has become apparent through the verification of these

96 predictions that current state-of the art models still exhibit persistent and systematic

97 shortcomings due to an inadequate representation of unresolved processes.

98 Despite the continuing increase of computing power, which allows numerical weather and

99 climate prediction models to be run with ever higher resolution, the multi-scale nature of

100 geophysical fluids means that many important physical processes (e.g. tropical convection,

101 gravity wave drag, micro-physical processes) are still not resolved. Parameterizations of

102 sub grid-scale processes contain closure assumptions, and related parameters with inherent

103 uncertainties. Although increasing model resolution gradually pushes these assumptions

104 further down the spectrum of motions, it is realistic to assume that some form of closure

105 will be present in simulation models into the foreseeable future.

106 Moreover, for climate simulations, a decision must be made as to whether computational

107 resources should be used to increase the representation of sub grid physical processes or to build

108 a comprehensive Earth-System Model, by including additional climate components such as the

109 cryosphere, chemistry and biosphere. In addition, the decision must be made about whether

110 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. These tropical multi-scale processes need to resolve

114 small-scale processes such as convection in addition to capturing the large-scale response and

115 feedback. Many of the Coupled Model Intercomparison Project phase 5 (CMIP5) climate

116 models still do not properly simulate the MJO and convectively coupled waves (Hung et al.

117 2013).

118 Mathematical approaches to stochastic modeling rely on the assumption that a physical

119 system can be expressed in terms of variables of interest, and variables which one does not

120 want to explicitly resolve. In the mathematical literature this is usually referred to as the

121 operation of coarse graining and performed through the method of homogenization

122 (Papanicolaou and Kohler 1974, Gardiner 1985, Pavliotis and Stuart 2008). The goal is then

123 to derive an effective equation for the slow predictable processes and to represent the effect

124 of the now unresolved variables as random noise terms.

125 Such a thinking underlies the pioneering study of Hasselmann (1976), who split the coupled

126 ocean-atmosphere system into a slow ocean and fast weather fluctuation components and

127 subsequently derived an effective equation for the ocean circulation only. One finds that the

128 impact of the fast variables on the dynamics of the slow variables boils down to a

129 deterministic correction – a mean field effect sometimes referred to as noise-induced drift

130 or rectification – plus a stochastic component, which is a white random noise in the limit of

131 infinite time scale separation.

132 Many rigorous methods in subgrid-scale parameterization are based on the assumption of a scale

133 separation. Without a scale separation one needs to consider memory effects in the

134 parameterization scheme. Often, it is thought that traditional parameterizations require a gap in

the power spectrum between small (length) scale and large-scale processes, although this is not

necessary (see e.g. the discussion on scale-separation in Yano 2015). 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). An example for a simple

red noise model that has scale separation in the temporal sense, but not a gap in the power

spectrum is discussed in DelSole (2000).

In geophysical applications, there is often - but not always – a relationship between spatial and

temporal scales of variability, with fast processes associated to small scales and slow processes

associated to 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.

A great challenge to both, the deterministic and stochastic approach, is posed by the

representation of partially resolved processes (either in the time or space domain). 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 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 for the mass-flux formulation by Yano (2014). The range of scales on which a

physical process is only partially resolved is often referred to as the "gray zone" (e.g.

Gerard 2007). 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"). A big

3

158 advantage of the mathematically rigorous approach is that the subgrid-model is valid for

159 increasing spatial resolutions within a range of scales that is obtained as part of the

160 derivation.

161 Stochastic parameterization schemes are now routinely used by operational weather and climate

162 centers to make ensemble predictions from short-range to seasonal time scales (e.g., Berner et al.

163 2009, Weisheimer et al. 2014). Most ensembles suffer from underdispersion, which means that -

164 on average – the observed state is more often outside the cone of forecasts than can be

165 statistically justified. Stochastic perturbations introduce more diversity among the forecasts,

166 which helps to ameliorate this problem and result in more skillful ensemble forecasts.

167 A fundamental argument, that has been often overlooked, is that the merit of stochastic

168 parameterization goes far beyond providing uncertainty estimations for weather and climate

169 predictions, but is also needed for better representing the mean state (e.g., Sardeshmukh et al.

170 2001, Palmer 2001) and regime transitions (e.g., Williams et al. 2003, 2004, Birner and

171 Williams 2008, Christensen et al. 2015a) via inherent non-linear processes. This is especially

172 relevant for climate predictions, which have long-standing mean state errors, such as e.g., a

173 double intra-tropical convergence zone (e.g., Lin et al. 2007), and erroneous stratocumulus

174 cloud covers, which play a crucial role in the climate response to external forcing.

175 Mechanisms how Gaussian zero-mean fluctuations can change the mean state have been

176 discussed e.g. in Tompkins and Berner (2008) and Beena and von Storch (2009). The former

177 study introduces perturbations to the humidity field. They find that positive perturbations are

178 more likely to trigger a convective event than negative perturbations suppress convection. Beena

179 and von Storch (2009) investigate the ocean response to fluctuating air-sea fluxes. They find that

180 negative buoyancy anomalies are likely to trigger convection which in turn alters the existing

181   stratification, while positive anomalies sustain the existing stratification. Insofar as stochastic

182   parameterizations can change the mean state, they have the potential to affect the response to

183   changes in the external forcing (e.g., Seiffert and von Storch 2008). In mathematical terms, this

184   is the question how a stochastic forcing affects the invariant measure of a deterministic

185   dynamical system (Lucarini 2012) and how the climate response to such a forcing can be framed

186   as a problem of non-equilibrium statistical mechanics (Colangeli et al. 2012, 2014, Lucarini and

187   Sarno 2011, Lucarini et 2014a,).

188   The essential fact that a white-noise forcing with zero mean can lead to a non-linear or rectified

189   response and change the mean state is shown in Figure 1. Assume the unforced nonlinear

190   climate system can be simplified as a double-well potential (a). If the noise is sufficiently small

191   (denoted by short red arrows) and under appropriate initial conditions, the system will stay in the

192   deeper potential well and the associated probability density function of states will have a single

193   maximum (b). As the amplitude of the noise increases (long arrows in c), the system can

194   undergo a noise-induced transition and reach the secondary potential well. The resulting

195   probability density function (PDF) will exhibit two local maxima (d), signifying two different

196   climate regimes, rather than a single maximum, as in the small-noise scenario. Note, that the

197   stochastic forcing not only changes the variance, but also the mean. But even a linear system

198   characterized by a single potential when unforced can change the mean, if forced by

199   multiplicative or state-dependent white noise (e-h). The noise is called "multiplicative", if its

200   amplitude is a function of the state, which is denoted by the red errors of different length in

201   panel g. The noise-induced drift changes the single-well potential of the unforced system (e), so

202   that the effective potential including the effects of the multiplicative noise has multiple wells

203   (not shown) and the associated PDF becomes bimodal (h). Note, that in this example the shift in

204   the mean compared to the unforced PDF (f) is caused by the noise, which is referred to as

205   "noise-induced drift" (see e.g., Sardeshmukh et al. 2001, Berner 2005, Berner et al. 2005, Sura

206   et al. 2005).

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

208   • Estimating uncertainty in weather and climate predictions

209   • Reducing systematic model errors

210   • Triggering noise-induced regime transitions

211   • Capturing the response to changes in the external forcing

212   and should be applied in a systematic and consistent fashion, not only to weather, but also to

213   climate simulations.

214   Several studies have identified the assessment of the benefits of stochastic closure schemes as

215   key outstanding challenge in the area of mathematics applied to the climate system (Palmer

216   2001, 2012, Palmer and Williams 2008, Williams et al. 2013). For accessible reviews of

217   rigorous mathematical approaches applied to weather and climate, we refer to Penland

218   (2003a,b), Majda et al. (2008) and Franzke et al. (2015). The current study focuses on recent

219   successful applications of empirical and rigorous approaches to the subgrid-parameterization

220   problem in weather and climate models.

221   **2 Representing Uncertainty in Comprehensive Climate and Weather Models**

222   ***2.1 Adding uncertainty a posteriori: the stochastically perturbed parameterization tendency***

223   ***scheme and the stochastic kinetic-energy backscatter scheme***

224   Stochastic parameterizations are based on the notion that – as spatial resolution increases – the

225 method of averaging (Arnold 2001, Monahan and Culina 2011) is no longer valid and the

226 subgrid-scale variability should be sampled rather than represented by the equilibrium mean. In

227 addition, unrepresented interactions between unresolved subgrid-scale processes with the large-

228 scale flow might affect the resolved dynamics.

229 The former is addressed by the stochastically perturbed parameterization tendency (SPPT)

230 scheme, which perturbs the net tendencies of the physical process parameterizations

231 (convection, radiation, cloud physics, turbulence and gravity wave drag). One essential feature

232 for its success is that the noise is correlated in space and time. SPPT has a beneficial impact on

233 medium range, seasonal and climate forecasts (Buizza et al. 1999, Teixeira and Reynolds 2008,

234 Palmer et al. 2009, Weisheimer et al. 2014, Berner et al. 2015, Christensen et al. 2015b, Dawson

235 and Palmer 2015, Batté and Doblas-Reyes 2015)

236 The stochastic kinetic-energy backscatter scheme (SKEBS) aims to represent model uncertainty

237 arising from unresolved subgrid-scale processes and their interactions with larger scales by

238 introducing random perturbations to the streamfunction and potential temperature tendencies.

239 For this purpose, the scheme re-injects a small fraction of the dissipated energy into the resolved

240 flow. Originally developed in the context of Large Eddy Simulations (LES; Mason and

241 Thomson 1992), and applied to models of intermediate complexity (Frederiksen and Davies

242 1997), it was adapted by Shutts (2005) for Numerical Weather Prediction (NWP). Its beneficial

243 impact on weather and climate forecasts are reported e.g., in Berner et al. (2008, 2009, 2011,

244 2012, 2015), Bowler et al. (2008, 2009), Palmer et al. (2009), Doblas- Reyes et al. (2009),

245 Charron et al. (2010), Hacker et al. (2011), Tennant et al. (2011), Weisheimer et al. (2011,

246 2014), Romine et al. (2015), Sanchez et al. (2015), albeit Shutts (2013) criticizes the arbitrary

247 nature of some of the design features. Instead, he proposes a convective SKEBS (Shutts, 2015),

248   which introduces a phase relationship between flow and perturbations and adds additional

249   perturbations to the divergent flow.

250   While these schemes are motivated by physical reasoning and scheme parameters are

251   informed in some manner, for example by coarse-graining high-resolution output (Shutts

252   and Palmer 2007, Shutts and Callado Pallarès 2014) or comparison with observations

253   (Watson et al. 2015), the perturbations are essentially empirical constructs. For example,

254   the amplitude of the perturbations is typically determined as the value that satisfactorily

255   reduces the ensemble underdispersion. Obviously such an approach is only possible for

256   forecast ranges where verification is possible, such as for short-term, medium-range and

257   seasonal forecasts. A common criticism of this approach is that the improved skill is solely

258   the result of the increase in spread. However, Berner et al. (2015) found that the merits of

259   stochastic parameterization go beyond increasing spread and can account for structural

260   model uncertainty.

261   In the following examples, we show recent results that demonstrate the potential of

262   stochastic parameterizations to improve the mean state representation and variability as

263   well as the skill of seasonal forecasts.

264   First, we present recent results from the seasonal forecasting system at ECMWF. In the

265   simulations with stochastic parameterizations, excessively strong convective activity over

266   the Maritime Continent and the tropical Western Pacific is reduced, leading to smaller

267   biases in outgoing longwave radiation (Figure 2), cloud cover, precipitation and near-

268   surface winds (Weisheimer et al. 2014). The stochastic schemes also lead to an increase in

269   the frequency (Figure 3) and amplitude of MJO events. A reduction of excessive amplitudes

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270 in westward propagating convectively coupled waves in an earlier model version is reported

271 in Berner et al. 2012.

272 Another example of the positive impact of stochastic schemes is evident in climate

273 simulations with the Community Earth System Model (CESM). Compared to observations,

274 the modeled spectrum of average sea surface temperature in the Nino 3.4 region has three

275 times more power for periods between 2 and 4 years (Figure 4). SPPT markedly reduces the

276 temperature variability in this frequency range, leading to a much better agreement with

277 nature (Christensen et al., 2016). Interestingly, in these examples the benefit of adding

278 stochasticity consists of *reducing* excessive variability, which is a non-trivial response.

279 Along with the improvements of the model climate, stochastic perturbations also benefit

280 probabilistic forecast performance on seasonal timescales. This has been reported in a

281 number of studies using earlier versions of ECMWF's seasonal system (Berner at al. 2008,

282 Dobles-Reyes et al. 2009, Palmer at al. 2009) and recently been confirmed in the newest

283 version (Weisheimer et al. 2014) and in the EC-Earth system model (Batté and Doblas-

284 Reyes 2015). Figure 5 shows ensemble mean and spread in forecasts for Nino 3.4 area sea-

285 surface temperatures with the EC-Earth model, run at a standard horizontal resolution (SR,

286 ca. 60km for the atmospheric and ca. 100km for the ocean component) and a high

287 resolution (HR, ca. 40km for the atmospheric component and 25km for the ocean.) For both

288 resolutions, the introduction of SPPT perturbations increases the ensemble spread.

289 Furthermore, SPPT reduces the mean error in the standard resolution, but not as much as

290 moving to a higher resolution.

291 A number of studies have found evidence for stochasticity leading to noise-induced

292 transitions in mid-latitude circulation regimes, especially over the Pacific-North America

293   region (Jung et al. 2005, Berner et al. 2012, Dawson et al. 2015, Weisheimer et al. 2014).

294   These results suggest that stochastic parameterizations are also relevant for the prediction of

295   low-frequency features (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   Strictly, the first variant is not a stochastic parameterization, but an example for a multi-

307   model, since each ensemble member has a different climatology. However, since stochastic

308   parameter perturbations are routinely compared to fixed-parameter schemes, this section

309   discusses both.

310   While perturbed-parameter ensembles typically outperform unperturbed ensemble system

311   on 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   Here, an ensemble system considered statistically reliable when a predicted probability for

315   a particular event (e.g. temperature exceeding 17°C) compares well with the observed

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316   frequencies. Another limitation of this approach is that the parameter uncertainty estimates

317   are subjective, and information about parameter interdependencies is not included.

318   The following studies are examples for applications of the perturbed-parameter approach to

319   physical process parameterizations and perturbing the interface between different model

320   components. We start with results pertaining to perturbations in the atmospheric

321   component and move to those of other model components, such as land and ocean models,

322   which are especially relevant for climate applications.

323   A number of studies report on improved skill due to parameter perturbations to boundary

324   layer and convection schemes (Hacker et al. 2011, Reynolds et al. 2011). Recently, a

325   stochastic "eddy-diffusivity/ mass-flux" parameterization has been developed, (Suselj et al.

326   2014), which combines an eddy-diffusivity component with a stochastic mass-flux scheme.

327   The resulting scheme unifies boundary layer and shallow convection and was operationally

328   implemented in the operational Navy Global Environmental Model.

329   Christensen et al. (2015b) used an objective covariance estimate of parameter uncertainty

330   (Järvinen et al. 2012, Ollinaho et al. 2013) for four convection closure parameters and developed

331   both a fixed-parameter and a stochastically varying perturbation scheme. Both schemes

332   improved the forecast skill of the ensemble prediction system, with a larger impact observed for

333   the fixed perturbed parameter scheme (Figure 6, bottom). In addition, for some variables such as

334   wind at 850hPa, the schemes lead to a reduction in bias (Figure 6, top).

335   Recently, a body of work proposes stochastic approaches for another atmospheric

336   parameterization, namely non-orographic gravity waves (Lott et al. 2012, Lott and Guez 2013,

337   and de la Cámara and Lott 2015). Observational studies indicate that the gravity wave field is

338   very intermittent and only predictable in a statistical sense. Recently, de la Cámara et al. (2014)

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339 informed the free parameters of the stochastic gravity-wave scheme using momentum flux

340 measurements.

2.3 Uncertainty in land surface, ocean and coupled component models

342 Physical parameters of land surface models are often not well constrained by observations. A

343 recent study by MacLeod et al. (2015) introduced parameter perturbations to two key soil

344 parameters, and compared their impact with stochastic perturbations of the soil moisture

345 tendencies in seasonal forecasts with the ECMWF coupled model. Both the perturbed parameter

346 approach and the stochastic tendency perturbations improved the forecasts of extreme air

347 temperature for the European heat wave of 2003, through better representation of negative soil

348 moisture anomalies and the upward sensible heat flux.

349 Another source of uncertainty in land models stems from the land surface heterogeneity, which

350 impacts the surface heat fluxes in coupled models. The effect of representing variability

351 associated with land surface heterogeneity in vegetation has been investigated by Langan et al.

352 (2014). This stochastic parameterization retains the subgrid variability among different plant

353 functional types rather than using constant area weights for the computation of the surface heat

354 fluxes. First results with a single column model version of CESM reveal an increase in the

355 variability as well as larger extreme values in convective precipitation (Figure 7).

356 The coupled atmosphere-ocean system is very sensitive to fluctuations in the fluxes between its

357 component models. Air-sea fluxes of buoyancy, energy, and momentum vary on a vast range of

358 space and time scales, including scales that are too small or fast to be explicitly resolved by

359 global climate models. For example, convective clouds in the atmosphere will cause subgrid

360 fluctuations at the air-sea interface, in both the downward fresh water flux (through

361 precipitation) and the downward short-wave solar radiation. The response of the climate to

362   stochastic perturbations of the air-sea buoyancy flux is studied by Williams (2012) in a coupled

363   atmosphere-ocean model. The response is complex and involves changes to the oceanic mixed-

364   layer depth, sea-surface temperature, atmospheric Hadley circulation, and fresh water flux

365   across the sea surface (Figure 8). These findings suggest that the lack of representation of

366   stochastic subgrid variability in air-sea fluxes may contribute to some of the biases exhibited by

367   contemporary coupled climate models.

368   Since the buoyancy effects in the ocean are different from that in the atmosphere, the length

369   scale at which rotational effects become as important as gravity wave effects (also called the

370   Rossby deformation radius) is much smaller. Consequently, mesoscale eddies in state-of-the art

371   ocean models are still far from being resolved and are usually represented by traditional bulk

372   parameterizations (Gent and McWilliams 1990, Redi 1982). A recent study by Li and von

373   Storch (2013) computes the contributions from the mean and fluctuating component of heat flux

374   divergence in a high-resolution ocean model. The magnitude of the fluctuations is about one

375   order of magnitude larger than the mean component (Figure 9) suggesting that classical

376   parameterization significantly underestimate the total eddy flux. The fluctuating part, even

377   though having zero mean, can play an important role in generating large-scale low-frequency

378   variations and in shaping the mean oceanic circulation.

379   Juricke et al. (2013) and Juricke and Jung (2014) recently investigated the sensitivity of an

380   ocean-sea ice model to variations in the ice strength parameter. As this parameter is not

381   observable, large uncertainties remain in the choice of its value, although it is very important for

382   modeling sea ice drift. Varying this parameter stochastically results in changes to the mean sea

383   ice distribution as well as sea ice spread. Compared to perturbations of the atmospheric initial

384   conditions, the incorporation of additional stochastic ice strength perturbations leads to

385 considerably more sea ice spread in the central Arctic (Figure 10), which is a better match with

386 the observed uncertainties (Juricke et al. 2014).

387 ***2.4 Data Assimilation and Extreme Events***

388 The purpose of data assimilation is to combine observations with short term model-forecasts to

389 come up with a gridded and physically consistent estimate of the state of the atmosphere, also

390 called "analysis". One particular approach is to use ensemble forecasts as the first guess fields.

391 As such, ensemble data assimilation inherits the shortcomings of short-term ensemble

392 predictions, namely, the underdispersivness in the spread. Recent work has demonstrated that

393 the stochastic parameterizations that are beneficial for ensemble prediction, can also improve the

394 mean analysis (Isaksen et al. 2007, Houtekamer et al. 2009, Mitchell and Gottwald 2012,

395 Hamill and Whitaker 2011, Ha et al. 2015, Romine at al. 2015). In particular, Ha et al. 2015

396 showed that the benefits of including a stochastic parameterization go beyond a larger number of

397 observations passing quality control due to an increased spread. A cutting-edge frontier is the

398 use of memory effects in Kalman filter data assimilation schemes (O'Kane and Frederiksen

399 2012).

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

401 Most works focuses on a description of non-Gaussian subgrid-scale processes (Majda et al.

402 2009, Sardeshmukh and Sura 2009, Sura 2011, Sardeshmukh et al. 2015). Franzke (2012)

403 showed that his reduced stochastic model (see next section) captures the extremes of the full

404 model. Tagle et al. (2015) were the first to study the effect of the stochastic parameterizations in

405 a comprehensive climate model. They found that the stochastic parameterizations had a big

406 impact on the surface temperature mean and variability, but hardly changed the tail behavior.

407 This might be in part due to the fact that their stochastic schemes use Gaussian perturbations.

3 Systematic mathematical and statistical physics approaches

This section introduces systematic mathematical and statistical physics 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. Mathematical and Numerical implications of stochasticity

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

Moreover, stochastic systems require calculi and numerical schemes fundamentally different from the ones available to solve deterministic systems. The two most commonly used stochastic integral types are the Itô-integral (Itô 1951) and the Stratonovich-integral (Stratonovich 1966). When the fast processes of a continuous system are modeled by white noise – as is common for physical applications - the resulting stochastic model converges to a Stratonovitch stochastic differential equation (Wong and Zakai 1965, Papanicolaou and Kohler 1974, Gardiner 1985, Penland 2003a,b). Discrete systems converge to the Itô stochastic differential equation. Starting in the 1970s a solid framework of numerical methods for stochastic ordinary differential equations was developed (Rümelin 1982,

430 Kloeden and Platen 1992, Milstein 1995, Kloeden 2002). However, this has been extended

431 to high-order schemes only recently (Jentzen and Kloeden 2009, Weniger 2014). With

432 stochastic parameterizations becoming more common in weather and climate simulations, a

433 revision of the deterministic numerical schemes should be undertaken to ensure the

434 convergence of the numerical solutions.

435 *3.2 Homogenization and stochastic mode reduction*

436 Numerical weather and climate modeling can be seen as a model reduction problem. Because

437 we cannot numerically solve the full continuous equations, we have to truncate the equations at

438 some scale and then treat the unresolved processes in some smart way. A systematic approach

439 for the derivation of reduced order models from first principles is performed through the method

440 of homogenization or adiabatic elimination (Wong and Zakai 1965, Khas'minskii 1966, Kurtz

441 1973, Papanicolaou and Kohler 1974, Pavliotis and Stuart 2008). The fundamental idea is to

442 decompose the state vector into slow and fast components, represent the fast processes by a

443 stochastic term and derive analytically an effective equation for the slow, predictable modes.

444 Majda et al. (1999) and Majda et al., 2001 expanded this body of work by making additional

445 assumptions on the nonlinear self-interaction of the fast modes and coined the term "stochastic

446 mode reduction".

447 The stochastic mode reduction has been demonstrated to successfully model regime-behavior

448 and low-frequency variability for conceptual models of the atmosphere (Majda et al. 2003), the

449 barotropic vorticity (Franzke et al. 2005) and a quasi-geostrophic three-layer model on the

450 sphere with realistic orography (Franzke and Majda 2006). However, due to both, the shear

451 amount of analytical derivation and the compute-memory requirement in the numerical

452 implementation of the resulting equations, the stochastic mode reduction cannot be easily

453   applied to comprehensive climate models of arbitrary complexity. A possible way forward is to

454   apply the stochastic mode reduction locally at each gridpoint rather than globally (Dolaptchiev

455   et al. (2013 a,b).

456   These mathematical techniques are rigorously valid only in the limit of large time-scale

457   separation, although some studies report good empirical results, even when this condition is not,

458   or only partly met (Dozier and Tappert 1978a,b , Majda et al. 2003 2008, Franzke et al. 2005,

459   Franzke and Majda 2006). When the time scale separation between the fast and slow processes

460   is not too large, the picture of the parameterization as being constructed as the sum of a suitably

461   defined deterministic plus random corrections has to be amended to take memory effects into

462   account (e.g. Zwanzig 2001, Chekroun et al. 2015a,b). Unfortunately, the condition of scale

463   separation is typically not met in geophysical fluid dynamics applications (Sardeshmukh and

464   Penland 2015, Yano 2015, Yano et al. 2015) that poses limitations to the application of

465   homogenization. An alternative, which does not make any assumptions about time scale

466   separation and provides an explicit expression for the terms responsible for the memory effect is

467   proposed by Wouters and Lucarini (2012, 2013), who, instead, assume the presence of a weak

468   dynamical coupling between the fast and the slow scales of motion.

469   The question of which stochastic process is best suited to describe the nonlinear interactions of

470   the unresolved processes is an open question. While methods for Gaussian diffusion processes

471   are well known (Oppenheim 1975) it may be the case that other formulations like Lévy

472   processes are better suited to describe the underlying physics (Penland and Ewald 2008, Penland

473   and Sardeshmukh 2012, Hein et al. 2010, Gairing and Imkeller 2012, 2013, Thompson et al.

474   2015).

475   *3.3 Adaptation of Concepts from Statistical Physics to Weather and Climate*

476   The scale-aware representation of convection and clouds on high-resolution grids (1-50

477   km) has been a long-standing challenge for weather and climate models. Within a single

478   model column, convection is not uniquely determined by the resolved-scale processes,

479   and the distribution of possible realizations of subgrid-scale convection highly depends on

480   model resolution. Thus, to achieve scale-awareness, it is necessary to represent scale-

481   dependent convective fluctuations about the ensemble average response. In addition,

482   because of the lack of time-scale separation, a correct representation of convection across

483   scales requires memory of subgrid-states from previous time steps.

484   A novel approach to represent the fluctuations in an ensemble of deep convective clouds adapts

485   concepts from statistical mechanics (Craig and Cohen 2006). Based on this theory, a stochastic

486   parameterization of deep convection was developed to represent fluctuations of the subgrid

487   convective mass flux about statistical equilibrium (Plant and Craig 2008). This is especially

488   attractive for variable-resolution grids, since the statistics automatically adapt to the grid-

489   resolution. This approach was extended to shallow convective clouds by introducing a memory

490   effect arising from the correlation between the cloud mass fluxes and cloud lifetimes (Sakradzija

491   et al. 2015). Figure 11 shows histograms of the subgrid cloud-base mass flux in the stochastic

492   shallow cumulus cloud scheme and coarse-grained large-eddy simulation at different horizontal

493   resolutions. The histograms match closely and are scale-aware.

494   *3.4 Modeling convective processes by Markov chains and cellular automata*

495   Another way to introduce temporal memory and nonlocal effects is the use of Markov

496   chains and cellular automata. A Markov chain is a mathematical system that undergoes

497   transitions from one *discrete* state to another and the probabilities associated with the

498   various state changes are called transition probabilities. If observational data or high-

499 resolutions simulations are used to inform the transition probabilities, the Markov chains

500 are called data-driven.

501 An example for this approach is the "stochastic convective parameterization" which

502 describes the convective state of the entire model column as a discrete Markov chain.

503 (Khouider et al. 2010, Dorrestijn et al. 2013a,b, Gottwald et al. 2015). The system can only

504 reside in a few distinct convective states - clear sky, congestus, deep convection, stratiform

505 and shallow - and the random transitions from one state to another evolve as a Markov

506 chain. The horizontal domain of the numerical model is covered with a high-resolution

507 lattice (with typical lattice spacing of 100m to 1000m), and on each lattice node lives a

508 copy of the discrete stochastic process for the convective state (Figure 12). By averaging

509 over blocks of lattice nodes, convective area fractions and related quantities can be obtained

510 for spatial domains of arbitrary size. The resulting patterns and temporal behavior of the

511 area fractions are quite realistic. Furthermore, the formulation on a high-resolution lattice

512 (or microlattice) makes it possible to compute convective fractions for varying area sizes,

513 so that a parameterization based on these fractions is scale-adaptive.

514 The probabilities for transitions between the convective states can be obtained in different

515 ways. Khouider et al. (2010) and Frenkel et al. (2012) use physical insight to formulate

516 transition probabilities for the Markov chain model, Dorrestijn et al. (2013a,b, 2015) and

517 Gottwald et al. (2015) estimate the transition probabilities from convection-resolving LES,

518 following a method proposed by Crommelin and Vanden-Eijnden (2008). Peters et al.

519 (2013) use observations for their estimates, which notably differ from those based on

520 physical intuition.

521 A related approach are cellular automata which are often used as simple mathematical

522 models to simulate spatial self-organizational behavior such as convective organization A

523 cellular automaton describes the evolution of discrete states on a lattice grid. The states are

524 updated according to a set of rules based on the states of neighboring cells at the previous

525 time step. In addition to memory, cellular automata can allow for lateral communications

526 between neighboring grid boxes and thus introduce spatial correlations.

527 The idea of using cellular automata within NWP was first proposed by Palmer (2001) and

528 first applications used them as a quasi-stochastic pattern generator for SKEBS (Shutts 2005,

529 Berner et al. 2008). Bengtsson et al. (2013) pioneered the use of a cellular automaton for

530 the parameterization of convection. In traditional single-column parameterizations there is

531 no treatment of horizontal transports of heat, moisture or momentum due to convection. To

532 determine if the inclusion of lateral communication is beneficial, Bengtsson et al. (2013)

533 considered a two–way interaction between cellular automata and the traditional convection

534 parameterization. The cellular automaton evolves on a lattice with finer grid spacing than

535 the parent model and is randomly seeded in regions where CAPE exceeds a threshold. The

536 rules are linked to the updraft area fraction and large–scale wind. The scheme has been

537 shown to enhance the organization of convective squall-lines (Bengtsson et al. 2013) and

538 improves the skill of accumulated precipitation in a high-resolution ensemble prediction

539 system (Bengtsson and Körnich 2015).

540 *3.5 Climate Response in the presence of small-scale fluctuations*

541 While there is extensive work focusing on the response of the climate system to changes in

542 the external forcing, either natural - such as the forcing from a localized tropical heating as

543 it occurs in Nino - or anthropogenic - such as the forcing from increased greenhouse gases,

544   little attention has been given to the fact if and how the representation of the subgrid-scale

545   can alter that response. In the mathematical community, this is the topic of response theory

546   and the fluctuation-dissipation theorem (e.g., Marconi et al. 2008, Lacorata and Vulpiani

547   2007, Colangeli et al. 2011, Lucarini and Colangeli 2012, Colangeli and Lucarini 2014).

548   Seiffert and von Storch (2008) were the first to investigate the response of a climate model

549   to CO2-forcing in the presence of subgrid-scale fluctuations in atmospheric temperature,

550   divergence and vorticity. In their model, the strength of the global warming due to a CO2-

551   doubling is altered by up to 15% near the surface and up to 25% in the upper troposphere

552   (Figure 13) depending on the exact representation of the small-scale fluctuations. Applying

553   a stochastic model to their simulations, they found that the small-scale fluctuations change

554   the temperature response via a statistical damping that acts as a restoring force. In addition,

555   the small-scale fluctuations can affect feedback and interaction processes that are directly

556   coupled to an increase in CO2, thereby altering the CO2-related radiative forcing (Seiffert

557   and von Storch 2010).

558   The fluctuation-dissipation theorem (FDT) is concerned with the response of a system to

559   small changes in the forcing. In particular, it tries to relate the response to the natural

560   fluctuations in the system (Kubo 1966, Deker and Haake 1975, Hänggi and Thomas 1977,

561   Leith 1975, Risken 1984). In the atmospheric sciences, the FDT-operator is estimated from

562   model output, in particular the variances and covariances of the state variables at different

563   time lags. The so obtained empirical linear model is able to predict the response to chances

564   in the external forcing, such as signature from localized tropical heat forcing (Gritsun and

565   Branstator 2007, Gritsun et al. 2008).

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566   Achatz et al. (2013) argue that subgrid-scale parameterizations developed for a present day

567   climate, might no longer be accurate in a changing climate. They use the FDT to adjust the

568   subgrid-scale representation of the forced system. Figure 14 shows that a low-order model

569   with a subgrid-scale parameterization corrected by the FDT yields a better response in the

570   streamfunction variance than without the correction.

571   While some success of FDT-techniques to low-frequency climate modeling has been

572   demonstrated, some of the mathematical assumptions are not strictly met. Recent work has

573   expanded the mathematical underpinning by a more general formulation of the response theory

574   better suited for non-equilibrium systems (Ruelle 2009, Lucarini and Sarno 2011), and is able to

575   deliver climate projections using GCMs (Lucarini et al. 2014, Ragone et al. 2015).

576   *3.6 Statistical Dynamical Closure Theory*

577   Kraichnan (1959) first illustrated that renormalization of the statistical equations of fluid

578   motion can been used to produce self-consistent parameterizations of the subgrid turbulent

579   processes. It is on this basis that Frederiksen and Davies (1997) developed stochastic

580   parameterisations of subgrid turbulence in barotropic atmospheric simulations on the

581   sphere. The subgrid parameterisations consist of drain, backscatter and net eddy viscosities,

582   which are determined from the statistics of higher resolution closure simulations.

583   Implementation of this approach into an atmospheric GCM resulted in significantly

584   improved circulation and energy spectra (Frederiksen et al. 2003). These ideas were further

585   formulated and tested by Frederiksen (1999, 2012a,b), and O'Kane and Frederiksen (2008).

586   Frederiksen and Kepert (2006) then used the functional form of these closure approaches to

587   develop a zero-parameter stochastic modeling framework, where the eddy viscosities are

588   determined from higher resolution reference simulations. This is in contrast to typical

22

589   approaches in which heuristic subgrid parameterizations are developed based on some

590   physical hypothesis on the behavior of subgrid turbulence. This approach was successfully

591   applied to baroclinic geophysical simulations in Zidikheri and Frederiksen (2009, 2010a,b).

592   Recently, Kitsios et al. (2012, 2013) used the approach of Frederiksen and Kepert (2006) to

593   determine the eddy viscosities from a series of reference atmospheric and oceanic

594   simulations. The isotropized version of the subgrid eddy viscosities where then

595   characterized by a set of scaling laws. Large Eddy Simulations with subgrid models defined

596   by these scaling laws (solid lines in Figure 15) were able to reproduce the statistics of the

597   high resolution reference simulations (dashed lines in Figure 15) across all resolved scales.

598   These scaling laws further enable the subgrid parameterizations to be utilized more widely

599   as they remove the need to generate the subgrid coefficients from a reference simulation.

600   **Concluding Remarks**

601   In this article, we attempt to narrow the gap between the fields of numerical meteorological

602   models and applied mathematics in the development of stochastic parameterizations: on the one

603   hand geo-scientists are often unaware of mathematically rigorous results that can aid in the

604   development of physically relevant parameterizations, on the other hand mathematicians often

605   do not know about open issues in scientific applications that might be mathematically tractable.

606   Over the last decade or two, increasing evidence has pointed to the potential of this

607   approach, albeit applied in an *ad hoc* manner and tuned to specific applications. This is

608   apparent in the choices made at operational weather centers, where stochastic

609   parameterization schemes are now routinely used to represent model inadequacy better and

610   improve probabilistic forecast skill. Here, we revisit recent work that demonstrates that

611   stochastic parameterization are not only essential for the estimation of the uncertainty in

612   weather forecasts, but are also necessary for accurate climate and climate change

613   projections. Stochastic parameterizations have the potential to reduce systematic model

614   errors, trigger noise-induced regime transitions, and modify the response to changes in the

615   external forcing.

616   Ideally, stochastic parameterizations should be developed alongside the physical

617   parameterization and dynamical core development and not tuned to yield a particular model

618   performance, as is current practice. This approach is hampered by the fact that parameters

619   in climate and weather are typically adjusted ("tuned") to yield the best mean state and/or

620   the best variability. This can result in compensating model errors, which pose a big

621   challenge to model development in general, and stochastic parameterizations in particular.

622   A stochastic parameterization might improve the model from a process perspective, but its

623   decreased systematic error no longer compensates other model errors, resulting in an

624   overall larger bias (Palmer and Weisheimer 2011, Berner et al. 2012). Clearly, such

625   structural uncertainties need to be addressed in order to improve the predictive skills of our

626   models.

627   Mathematically rigorous approaches decompose the system-at-hand into slow and fast

628   components. They focus on the accurate simulation of the large, predictable scales, while only

629   the statistical properties of the small, unpredictable scales need to be captured. One finds that the

630   impact of the fast variables on the dynamics of the slow variables boils down to a deterministic

631   correction plus a stochastic component. This immediately points to the fact that the classical

632   parameterization approach, which is only based upon averaged properties, is insufficient.

633   Understanding the deterministic correction term in physical terms will shed light on the impact

634   of stochastic parameterizations on systematic model errors and, hopefully, compensating model

635 errors.

636 Recent findings from such rigorous derivations suggest that when the time scales of the

637 processes we need to parameterize are not very different from those of the explicitly resolved

638 dynamics – if we are in a grey zone - memory terms can become important. This is especially

639 relevant for developing scale-aware parameterizations, where it is difficult to control the time

640 scale separation as the spatial resolution is altered.

641 Of course, the stochastic approach is not a panacea for the subgrid-scale parameterization

642 problem and persistent model biases. Stochastic approaches must complement

643 developments in the deterministic physical process parameterizations and dynamical core.

644 Nevertheless, it is our conviction, that basing stochastic parameterizations on sound

645 mathematical and statistical physics concepts will lead to substantial improvements in our

646 understanding of the Earth system as well as increased predictive capability in next

647 generation weather and climate models.

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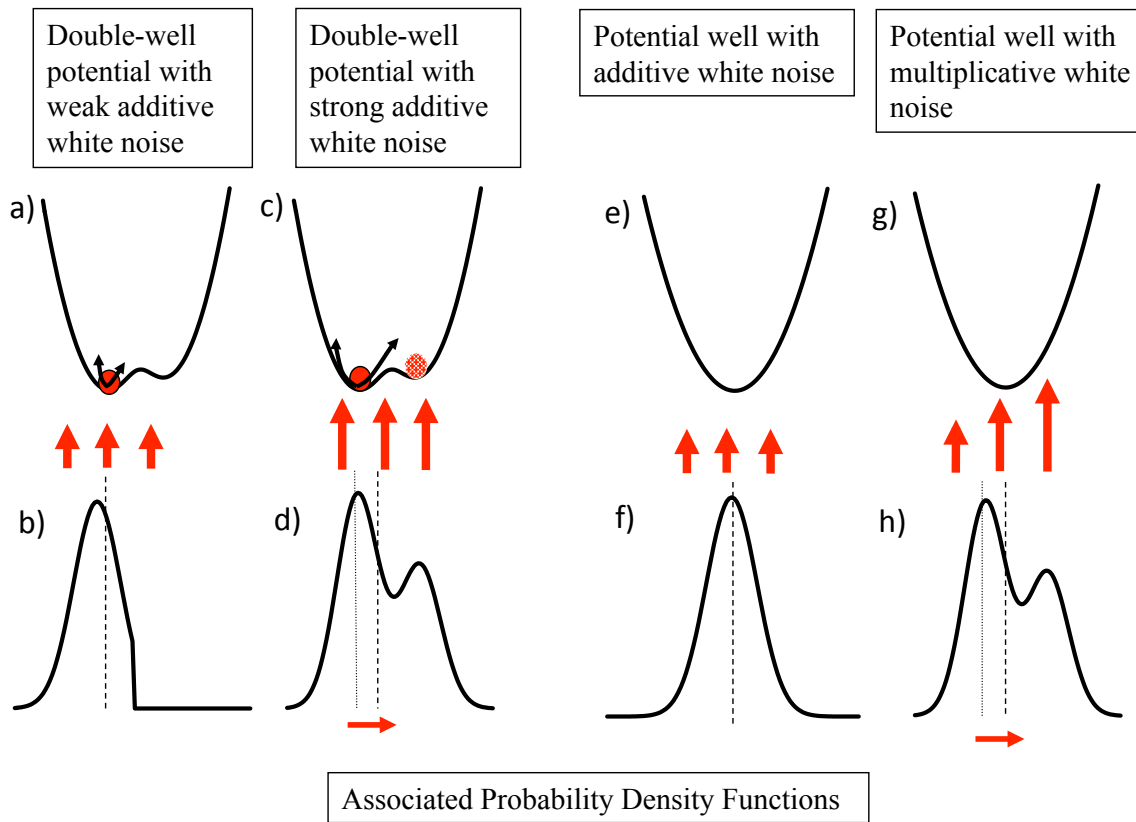
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Figure 1: System characterized by a,c) double-potential or e,g) single-potential well and their associated probability density functions (PDFs). If the noise is sufficiently small (a) and under appropriate initial conditions, the system will stay in 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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OLR   bias   DJF   1981-2010
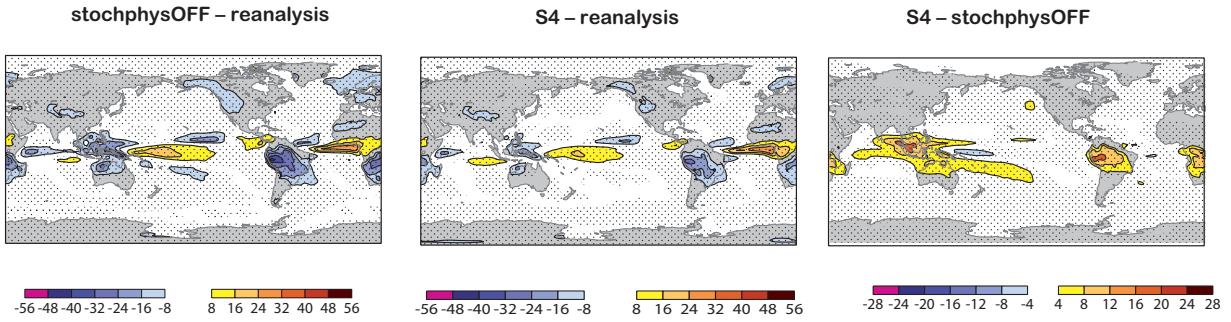
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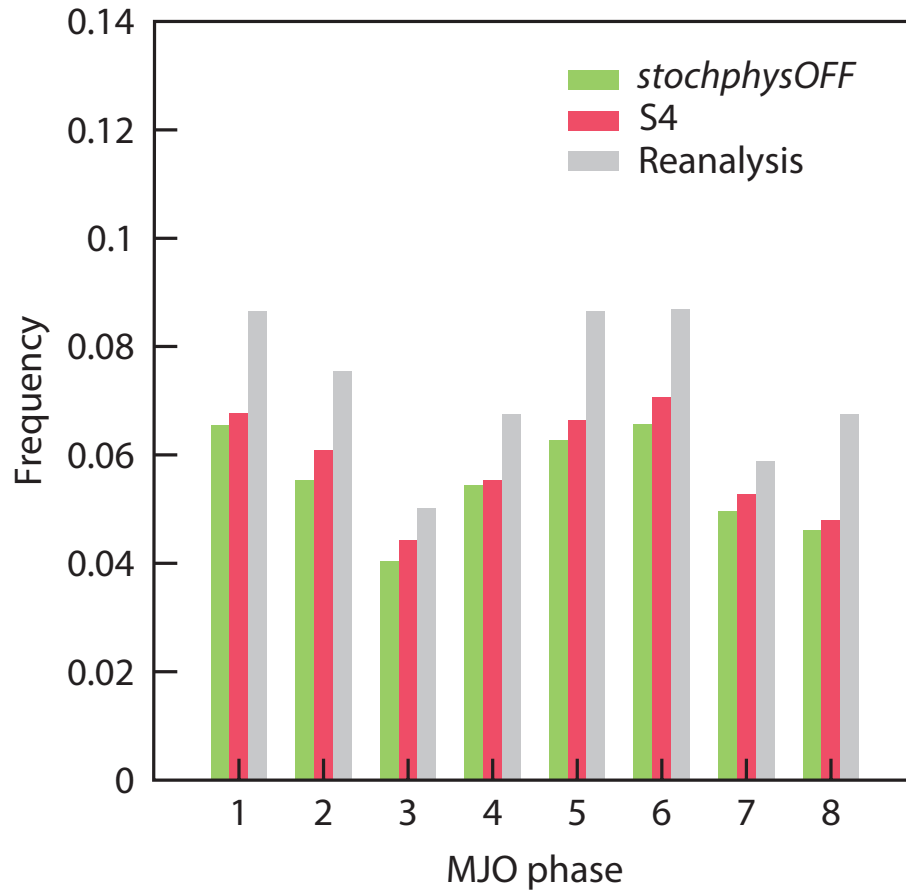
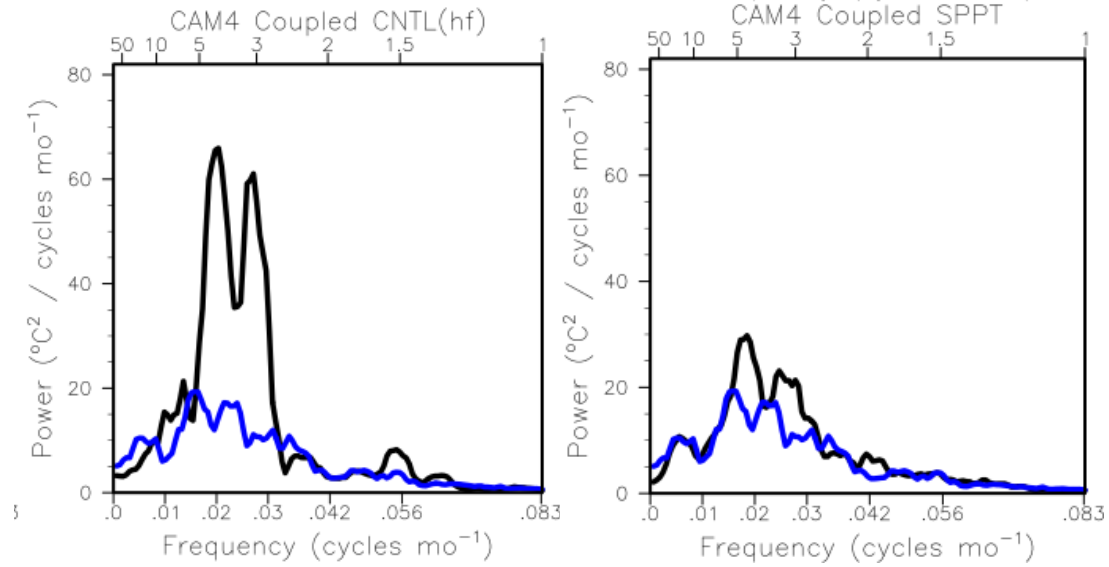Figure 3: Relative frequencies of MJO events in each of the eight MJO phases. From Weisheimer et al. (2014).

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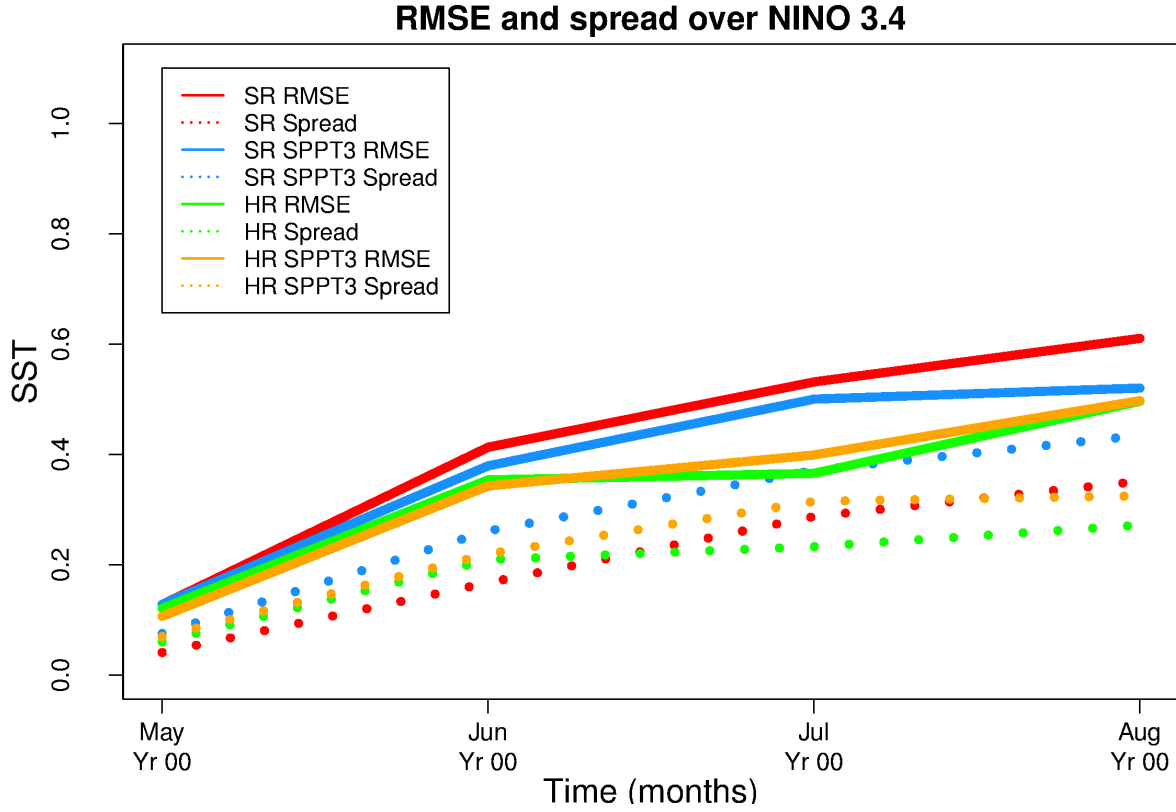
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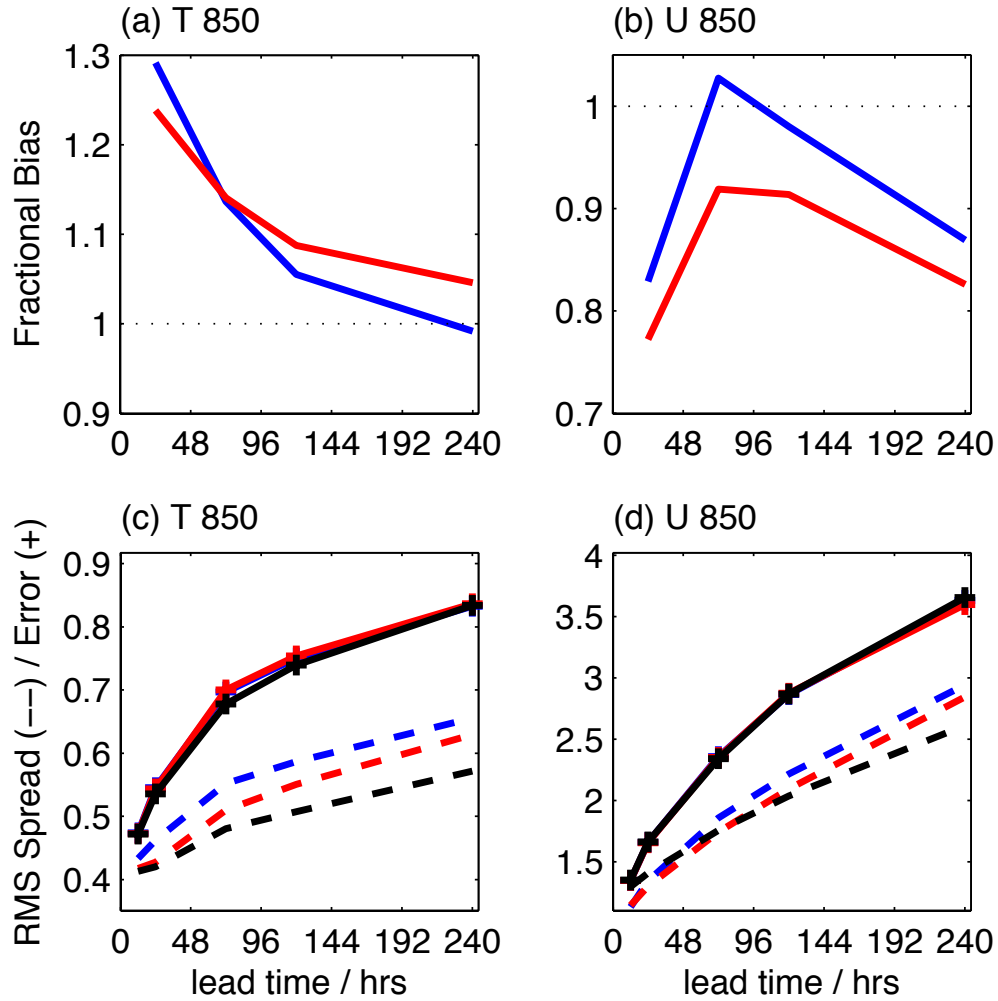
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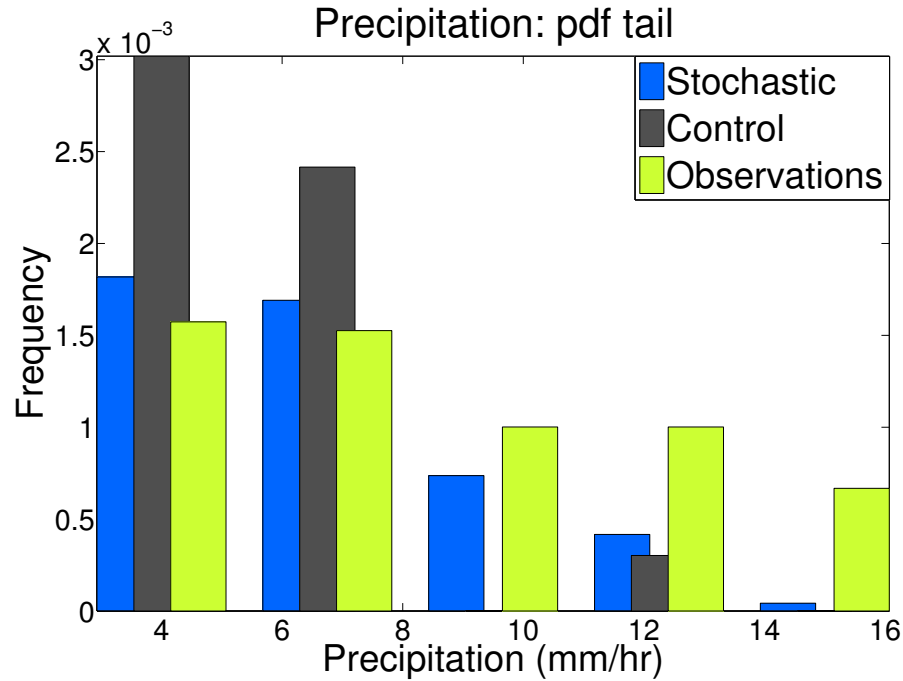
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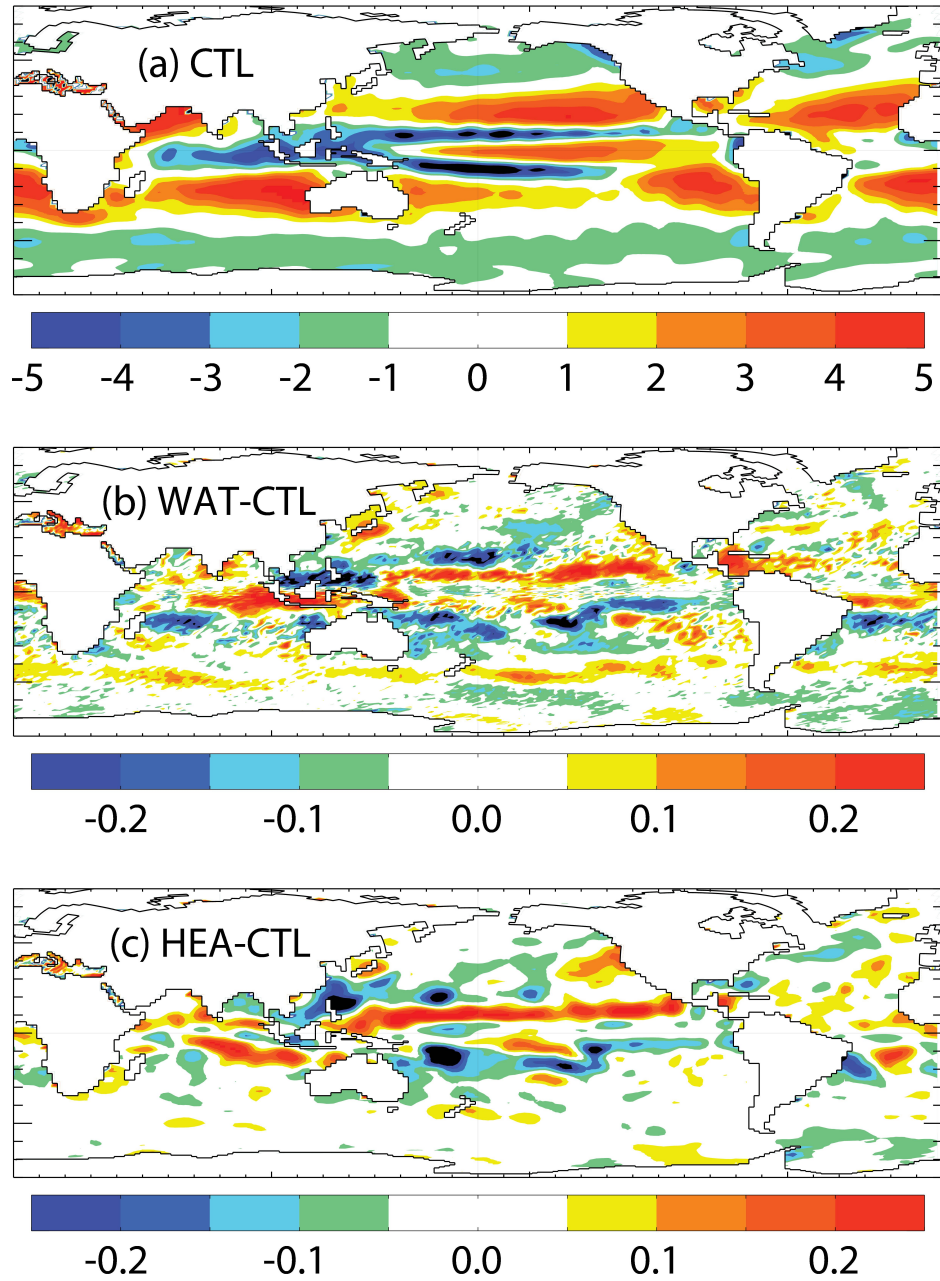
Figure 8: Maps of the century-mean net upward water flux (mm/day) at the sea surface in (a) a control integration of a coupled climate model. (b) Difference from the control for an experiment in which the net fresh water flux across the air–sea interface is stochastically perturbed before being passsed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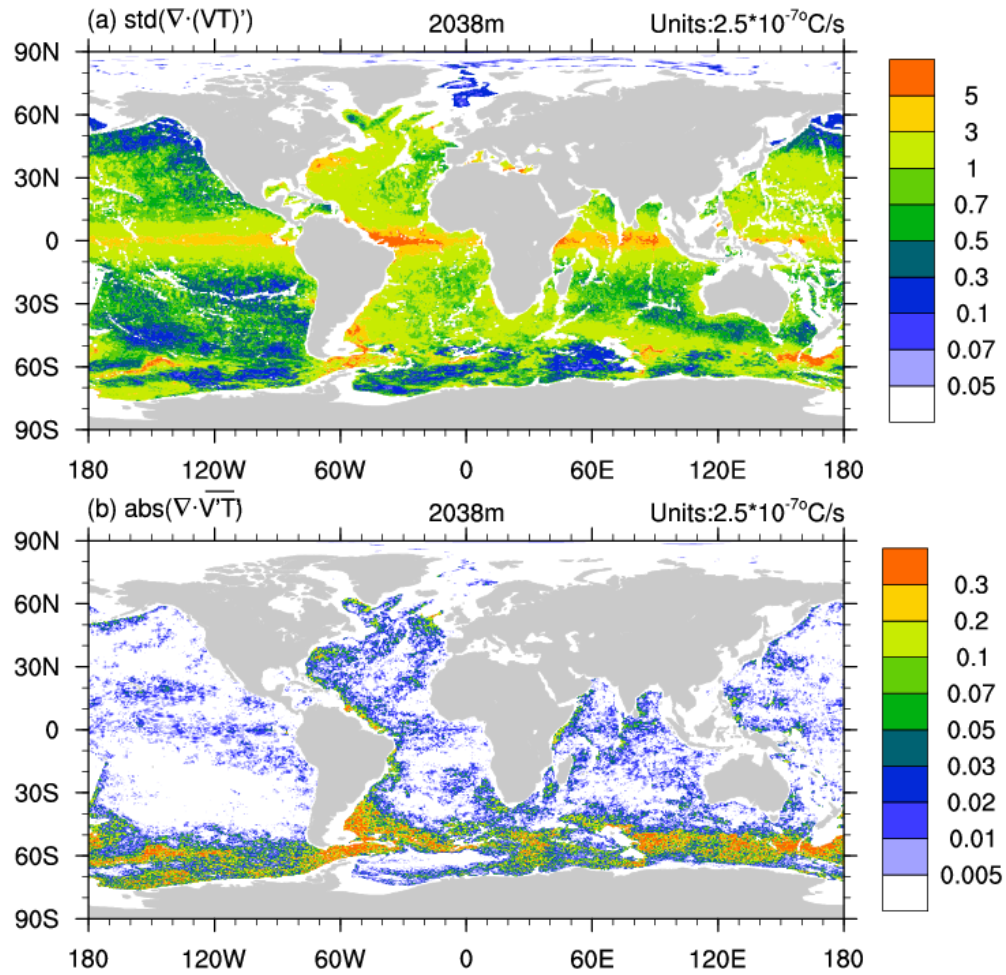e from the control for an experiment in which the net heat flux across the air–sea interface is stochastically perturbed before being passsed to the ocean. From Williams (2012).

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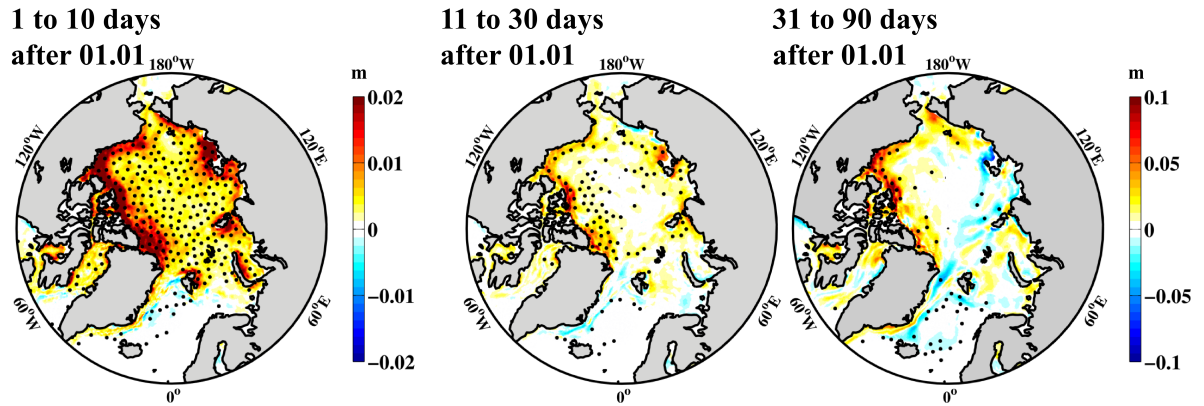
STD difference STOINI-INI

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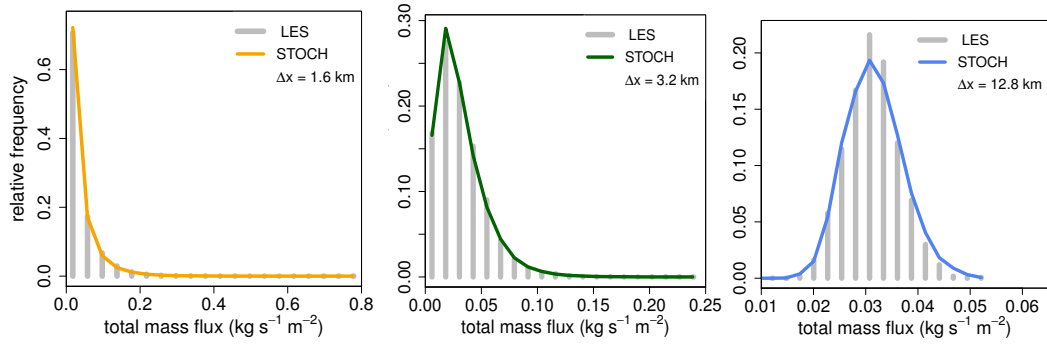
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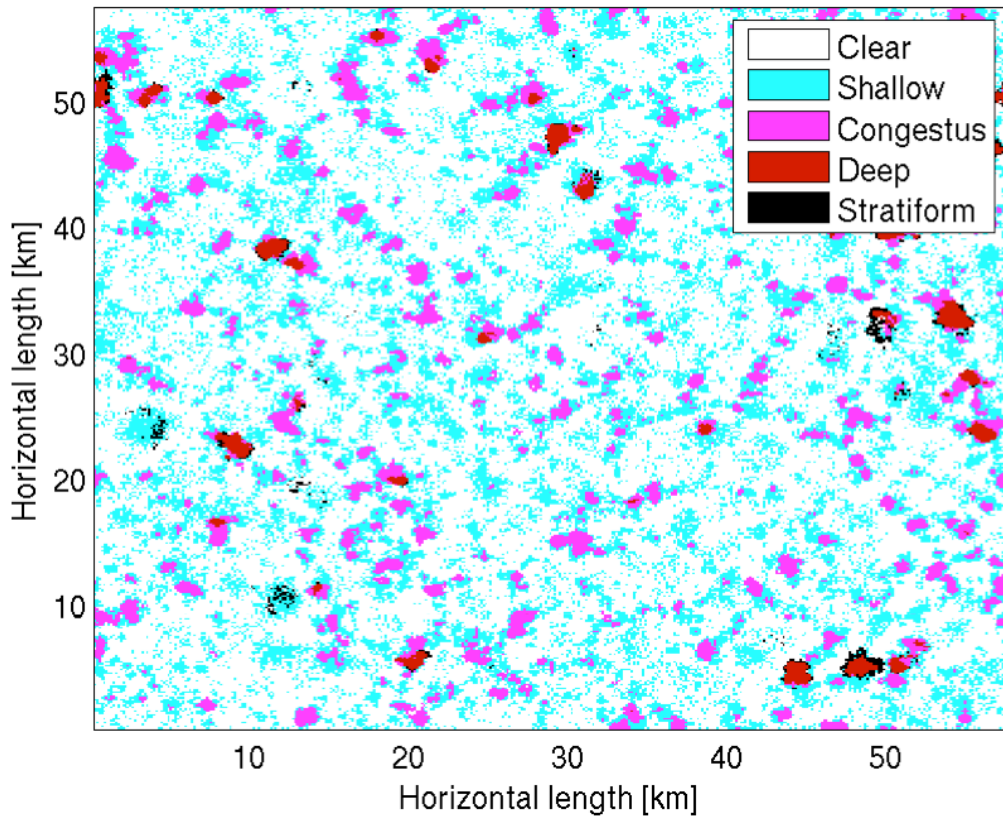
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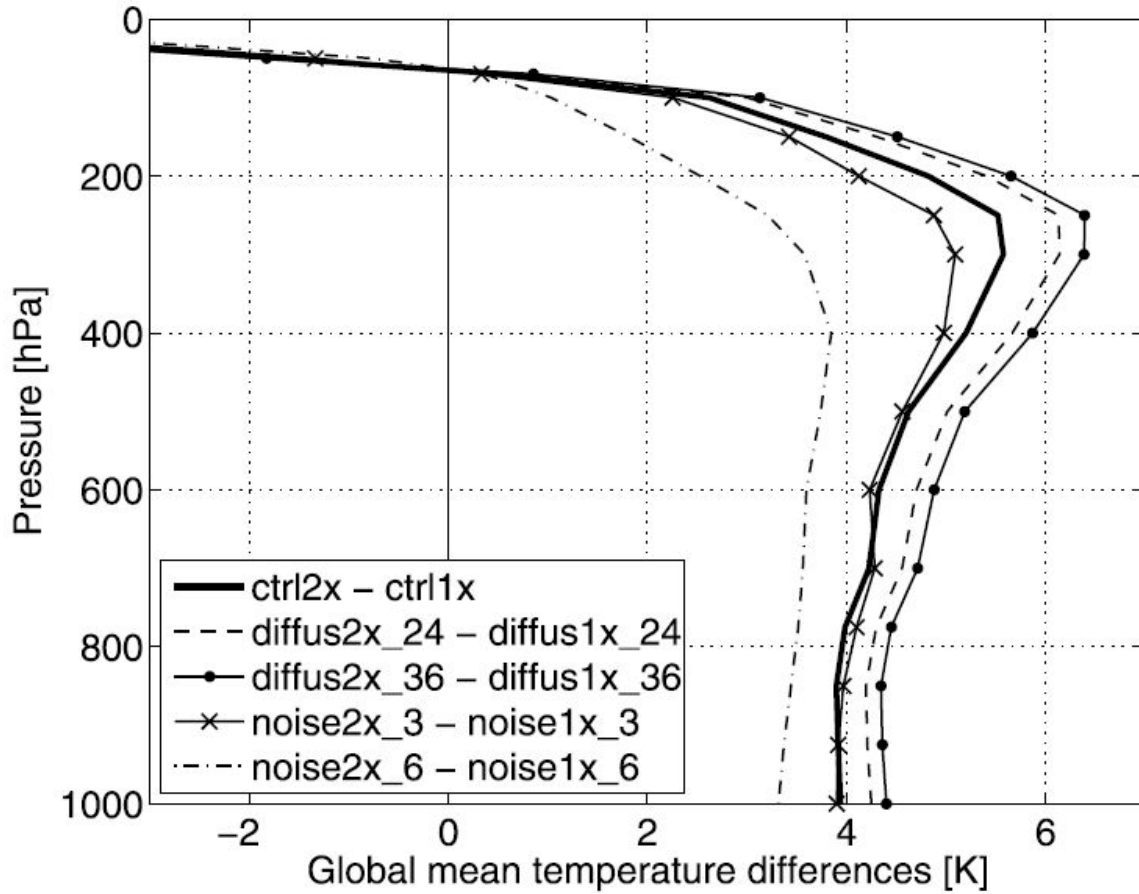
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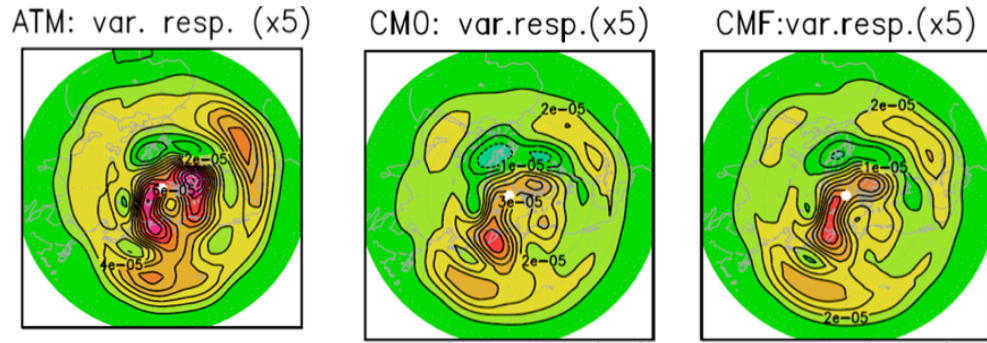
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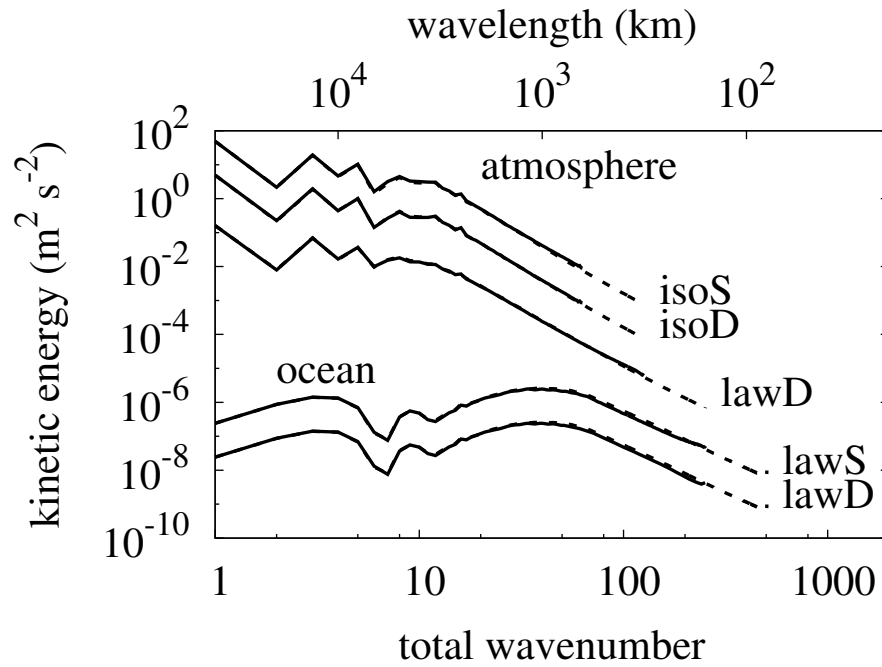
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