

Stochastic climate theory and modeling

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1	Stochastic Climate Theory and Modelling
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Abstract

Stochastic methods are a crucial area in contemporary climate research and are increasingly being used in 13 comprehensive weather and climate prediction models as well as reduced order climate models. Stochastic 14 methods are used as subgrid-scale parameterizations as well as for model error representation, uncertainty 15 quantification, data assimilation and ensemble prediction. The need to use stochastic approaches in weather 16 and climate models arises because we still cannot resolve all necessary processes and scales in comprehensive 17 numerical weather and climate prediction models. In many practical applications one is mainly interested in 18 the largest and potentially predictable scales and not necessarily in the small and fast scales. For instance, 19 reduced order models can simulate and predict large scale modes. Statistical mechanics and dynamical systems 20 21 theory suggest that in reduced order models the impact of unresolved degrees of freedom can be represented by suitable combinations of deterministic and stochastic components and non-Markovian (memory) terms. 22 Stochastic approaches in numerical weather and climate prediction models also lead to the reduction of model 23 biases. Hence, there is a clear need for systematic stochastic approaches in weather and climate modelling. In 24 this review we present evidence for stochastic effects in laboratory experiments. Then we provide an overview of 25 stochastic climate theory from an applied mathematics perspectives. We also survey the current use of stochastic 26 methods in comprehensive weather and climate prediction models and show that stochastic parameterizations 27 have the potential to remedy many of the current biases in these comprehensive models. 28

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²⁹ 1 Introduction

The last few decades have seen a considerable increase in computing power which allows the simulation of 30 numerical weather and climate prediction models with ever higher resolution and the inclusion of ever more 31 physical processes and climate components (e.g. cryosphere, chemistry). Despite this increase in computer 32 power many important physical processes (e.g. tropical convection, gravity wave drag, clouds) are still not 33 or only partially resolved in these numerical models. Despite the projected exponential increase in computer 34 power these processes will not be explicitly resolved in numerical weather and climate models in the foreseeable 35 future^{120,171}. For instance, Dawson et al.²⁴ have demonstrated using the ECMWF integrated forecast system 36 that extremely high resolutions (T1279, which corresponds to a grid spacing of about 16km) are required to 37 accurately simulate the observed Northern hemispheric circulation regime structure. This resolution, typical 38 for limited area weather and climate models used for short term prediction, remains unfeasible for the current 39 generation of high resolution global climate models due to computational and data storage requirements. Hence, 40 these missing processes need to be parameterized, i.e. they need to be represented in terms of resolved processes 41 and scales¹⁵³. This representation is important because small-scale (unresolved) features can impact the larger 42 (resolved) scales^{84,162} and lead to error growth, uncertainty and biases. 43

At present, these parameterizations are typically deterministic, relating the resolved state of the model to a 44 unique tendency representing the integrated effect of the unresolved processes. These "bulk parameterizations" 45 are based on the notion that the properties of the unresolved subgrid-scales are determined by the large-scales. 46 However, studies have shown that resolved states are associated with many possible unresolved states^{22,144,167}. 47 This calls for stochastic methods for numerical weather and climate prediction which potentially allow a proper 48 representation of the uncertainties, a reduction of systematic biases and improved representation of long-term 49 climate variability. Furthermore, while current deterministic parameterization schemes are inconsistent with 50 the observed power-law scaling of the energy spectrum^{5,142} new statistical dynamical approaches that are un-51 derpinned by exact stochastic model representations have emerged that overcome this limitation. The observed 52 power spectrum structure is caused by cascade processes. Recent theoretical studies suggest that these cascade 53 processes can be best represented by a stochastic non-Markovian Ansatz. Non-Markovian terms are necessary 54 to model memory effects due to model reduction¹⁹. It means that in order to make skillful predictions the 55 model has to take into account also past states and not only the current state (as for a Markov process). 56

We first review observational evidence of stochasticity in laboratory geophysical fluid experiments (section 2), then discuss stochastic climate theory in fast-slow systems (system 3). In section 4 we present statistical physics approaches and in section 5 we review the current state of stochastic-dynamic weather and climate modelling. We close with an outlook and challenges for the future of weather and climate modelling (section 6).

⁶¹ 2 Laboratory Evidence of Stochasticity

Research on the climate system is somewhat hindered by the obvious difficulties of performing reproducible experiments on the atmosphere and ocean in different parameter regimes. For example, an optical physicist studying the nonlinear response of isolated atoms to intense electromagnetic waves can easily change the incident wavelength¹¹⁰. In contrast, climate scientists cannot (and arguably should not!) change the rotation rate of the planet or the intensity of the incoming solar radiation. To some extent, numerical simulations come to the rescue, by allowing us to perform virtual experiments. However, the grid spacing in climate models is orders of magnitude larger than the smallest energized scales in the atmosphere and ocean, introducing biases.

Fortunately, there is another option available to us. It is possible to exploit dynamical similarity³⁰ to study analogues of planetary fluid flow in bespoke laboratory experiments. The traditional set-up is the classic rotating annulus, which has been used for decades to study baroclinic instability and other large-scale phenomena⁶¹. Recent observations of small-scale inertia-gravity waves embedded within a large-scale baroclinic wave^{85,172,173} have allowed the scale interactions between these two modes to be studied in a laboratory fluid for the first

time. The experimental apparatus consists of a two-layer isothermal annulus forced by a differentially rotating 74 lid, which drives a shear across the internal interface and represents the mid-latitude tropospheric wind shear. 75 The large-scale baroclinic wave in these laboratory experiments exhibits regime behavior, equilibrating at 76 finite amplitude with a zonal wavenumber of typically 1, 2, or 3. These simple wave modes are regarded as 77 prototypes of the more complicated regime behavior in the atmosphere, such as mid-latitude blocking^{160,164}. 78 A notable finding from repeated experiments using this apparatus is that small-scale inertia-gravity waves can 79 induce large-scale regime transitions, despite the separation of wavelengths by an order of magnitude 168 . An 80 example of this process is illustrated in Figure 1. A wavenumber 2 mode without co-existing inertia-gravity 81 waves (upper row) remains a wavenumber 2 mode indefinitely, drifting around the annulus with the zonal-mean 82 flow. In contrast, with the same parameter values, a wavenumber 2 mode with co-existing inertia-gravity waves 83 (lower row) is found to have a finite probability of transitioning to a wavenumber 1 mode. The amplitude of 84 the inertia-gravity waves is controlled here without directly affecting the large-scale mode, by slightly varying 85 the interfacial surface tension between the two immiscible fluid layers. 86

The laboratory transitions discussed above are reminiscent of noise-induced transitions between different 87 equilibrium states in a meta-stable dynamical system 158 . To test this interpretation, a quasi-geostrophic nu-88 merical model that captures the meta-stability of the large-scale flow in the rotating annulus¹⁷⁴ was run with 89 and without weak stochastic forcing added to the potential vorticity evolution equation for each fluid layer. 90 The stochastic forcing was an approximate representation of the inertia-gravity waves, which are inherently 91 ageostrophic and are therefore forbidden from the quasi-geostrophic model. Consistent with the laboratory 92 experiments, only when the noise term was activated did the numerical simulations exhibit large-scale wave 93 transitions in the equilibrated flow¹⁶⁹. In further numerical experiments, the noise was found to be able to 94 influence wavenumber selection during the developing baroclinic instability. 95

In summary, the above laboratory experiments constitute the first evidence in a real fluid that small-scale 96 waves may trigger large-scale regime transitions. In a numerical model in which the small-scale waves were 97 absent, the transitions were captured through the addition of stochastic noise. Note that the small-scale waves 98 satisfy the dispersion relation for inertia-gravity waves and are therefore coherent in space and time, and yet 99 apparently they are 'sensed' by the large-scale flow as if they were random fluctuations. These results have led 100 to a possible interpretation of sudden stratospheric warmings as noise-induced transitions⁹. Furthermore, these 101 laboratory results help to motivate the development of stochastic parameterizations in climate models and a 102 more general development of stochastic climate theory. 103

¹⁰⁴ **3** Stochastic Climate Theory

Climate is a multi-scale system in which different physical processes act on different temporal and spatial 105 $scales^{69}$. For instance, on the micro-scale are turbulent eddies with time scales of seconds to minutes, on 106 the meso-scale is convection with time scales of hours to days, on the synoptic scale are mid-latitude weather 107 systems and blocking with time scales from days to weeks, on the large-scale are Rossby waves and teleconnection 108 patterns with time scales of weeks to seasons. And there is the coupled atmosphere-ocean system with time 109 scales of seasons to decades. The crucial point here is that all these processes acting on widely different temporal 110 and spatial scales, interact with each other due to the inherent nonlinearity of the climate system. We have 111 shown an illustrative laboratory example for this in the previous section. 112

For many practical applications we are only interested in the processes on a particular scale and not in the detailed evolution of the processes at smaller scales. Often the scales of interest are linked to inherently predictable processes, while the smaller scales processes are unpredictable. For instance, in the above laboratory experiment we are interested in the regime behavior and not in the detailed evolution of the inertia–gravity waves. In numerical simulations the fastest scales, which are typically also the smallest scales, use up the bulk of computing time, slowing down the computation of the processes of actual interest. In numerical weather and climate prediction many of the small scale processes are currently not explicitly resolved and won't be in the ¹²⁰ foreseeable future. This neglect of these processes can lead to biases in the simulations. Because of that the ¹²¹ unresolved processes need to be parameterized as demonstrated in the previous section.

Stochastic climate theory is based on the concept of scale separation in space or time. Hasselmann⁵⁶ was 122 the first to propose to split the state vector \vec{z} into slow climate components \vec{x} and fast weather fluctuations \vec{y} 123 and then to derive an effective equation for the slow climate variables only. In this equation the effect of the 124 now unresolved variables is partially represented as a noise term. The physical intuition behind this idea is, 125 for example, that the aggregated effect of 'fast' weather fluctuations drives fluctuations in the 'slower' ocean 126 circulation. To first order such a model can explain the 'red' spectrum of oceanic variables 36,64 . It has to be 127 noted that there is no scale separation in the climate system. This lack of time-scale separation introduces 128 non-Markovian (memory) effects and complicates the derivation of systematic parameterizations. 129

Rigorous mathematical derivations for this approach have been provided by Gottwald and Melbourne⁵², Khasminsky⁶⁶, Kurtz⁷⁶, Melbourne and Stuart¹⁰¹, Papanicolaou¹²⁴, Pavliotis and Stuart¹²⁵. For accessible reviews see Givon et al.⁵⁰ and the text book by Pavliotis and Stuart¹²⁵. This approach has been applied to climate models by Majda and coworkers^{29,37,38,89–94,96}. Climate models have the following general functional form

$$d\vec{z} = \left(\tilde{F} + \tilde{L}\vec{z} + \tilde{B}(\vec{z}, \vec{z})\right)dt\tag{1}$$

where \tilde{F} denotes an external forcing, \tilde{L} a linear operator and \tilde{B} a quadratic nonlinear operator. Eq. (1) constitutes the form of the dynamical cores of weather and climate prediction models.

Now splitting the state vector \vec{z} into slow \vec{x} and fast \vec{y} components (which amounts to assuming a time scale separation) and assuming that the nonlinear self-interaction of the fast modes $\tilde{B}(\vec{y}, \vec{y})$ can be represented by a stochastic process^{37,38,89,90} leads to a stochastic differential equation. The stochastic mode reduction approach^{37,38,89,90} then predicts the functional form of reduced climate models for the slow variable \vec{x} alone:

$$d\vec{x} = (F + L\vec{x} + B(\vec{x}, \vec{x}) + M(\vec{x}, \vec{x}, \vec{x})) dt + \sigma_A d\vec{W}_A + \sigma_A(\vec{x}) d\vec{W}_M$$
(2)

Structurally new terms are a deterministic cubic term which acts predominantly as nonlinear damping and both additive and multiplicative (state-dependent) noise terms. The fundamentals of stochastic processes and calculus are explained in Box 1. The multiplicative noise and the cubic term stem from the nonlinear interaction between the resolved and unresolved modes³⁷.

The above systematic procedure allows also a physical interpretation of the new deterministic and stochastic terms³⁷. The additive noise stems both from the nonlinear interaction amongst the unresolved modes and the linear interaction between resolved and unresolved modes³⁷.

BOX 1

STOCHASTIC PROCESSES

In contrast to deterministic processes stochastic processes have a random component. See the books by Lemons⁸⁶ and Gardiner⁴⁹ for intuitive introductions to stochastic processes. Typically stochastic processes are driven by white noise. White noise is a serially uncorrelated time series with zero mean and finite variance 49 .

A stochastic differential equation (SDE) is a combination of a deterministic differential equation and a stochastic process. In contrast to regular calculus, stochastic calculus is not unique; i.e. different discretizations of its integral representation lead to different results even for the same noise realization. The two most important

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calculi are Ito and Stratonovich. See details in Gardiner⁴⁹. The physical difference is that Ito calculus has uncorrelated noise forcing while Stratonovich allows for finite correlations between noise increments. Hence, physical systems have to be typically approximated by Stratonovich SDEs. On the other hand, it is mathematically straightforward to switch between the two calculi. So one only needs to make a decision at the beginning which calculus is more appropriate for modeling the system under consideration and can then switch to the mathematically more convenient form.

SDEs describe systems in a path wise fashion. The Fokker-Planck equation (FPE) describes how the probability distribution evolves over time⁴⁹. Thus, SDEs and the FPE offer two different ways at looking at the same system. The parameters of SDEs and their corresponding FPE are linked; thus, one can use the FPE to estimate the parameters of the corresponding $SDE^{3,146}$

Multiplicative (or state-dependent) noise is important for deviations from Gaussianity and thus extremes. 149 The intuition behind multiplicative noise is as follows: On a windless day the fluctuations are very small, 150 whereas on a windy day not only is the mean wind strong but also the fluctuations around this mean are large; 151 thus, the magnitude of the fluctuations dependent on the state of the system. 152

The first practical attempts at stochastic climate modelling were made using Linear Inverse Models (LIM) 153 127,128,166,176 and dynamically based linear models with additive white noise forcing 26,27,34,35,179. These 154 approaches linearise the dynamics and then add white noise and damping¹⁶⁶ in order to make the models 155 numerically stable (i.e. the resulting linear operator should only have negative eigenvalues to ensure stability 156 and reliasability of the solutions). While these models have encouraging predictive skill, especially for ENSO, 157 they can only produce Gaussian statistics and, thus, are less useful for predictions of high impact weather. 158

Recently there are encouraging attempts in fitting nonlinear stochastic models to data. These include multi-159 level regression^{70,74}, fitting the parameters via the Fokker-Planck equation^{3,146}, stochastic averaging^{23,103}, 160 optimal prediction^{18,154} or Markov Chains²¹. Most of the previous approaches fitted the parameters of the 161 stochastic models without taking account of physical constraints, e.g. global stability. Many studies linearized 162 the dynamics and then added additional damping to obtain numerically stable models 1,2,166,179 . Majda et al. 96 163 developed the nonlinear normal form of stochastic climate models and also physical constraints for parameter 164 estimation. Recent studies use these physical constraints to successfully derive physically consistent stochastic 165 climate models 57,97,126166

Most of the above approaches are based on an implicit assumption of time scale separation. However, the 167 climate system has a spectrum with no clear gaps which would provide the basis of scale separation and the 168 derivation of reduced order models. Such a lack of time scale separation introduces memory effects into the 169 truncated description. Memory effects mean that the equations become non-Markovian and that also past states 170 need to be used in order to predict the next state. This can be explained by considering the interaction between 171 a large-scale Rossby wave with a smaller scale synoptic wave. At some location the Rossby wave will favor 172 the development of the synoptic wave. Initially this synoptic wave grows over some days without affecting the 173 Rossby wave. Once the synoptic wave has reached a sufficient large amplitude it will start affecting the Rossby 174 wave. Now in a reduced order model only resolving the Rossby wave but not the synoptic wave this interaction 175 cannot be explicitly represented. However, because the Rossby wave initially triggered the synoptic wave which 176 177 then in turn affects it some days later, this can be modeled with memory terms which takes into account that

the Rossby wave has triggered at time t_0 an anomaly which will affect it at some later time t_n .

Recently, Wouters and Lucarini¹⁷⁷ have proposed to treat comprehensively the problem of model reduction in 179 multi-scale systems by adapting the Ruelle response theory^{136,137} for studying the effect of the coupling between 180 the fast and slow degrees of freedom of the system. This theory has previously been used in a geophysical context 181 to study the linear and nonlinear response to perturbations^{87,88}, which also allows climate change predictions. 182 This approach is based on the *chaotic hypothesis*⁴⁸ and allows the general derivation of the reduced dynamics of 183 the slow variables able to mimic the effect of the fast variables in terms of matching the changes in the expectation 184 values of the observables of the slow variables. The ensuing parametrization includes a deterministic correction, 185 which is a mean field result and corresponds to linear response, a general correlated noise and a non-Markovian 186 (memory) term. These results generalize Eq. (2). In the limit of infinite time-scale separation, the classical 187 results of the averaging method is recovered. Quite reassuringly, the same parametrizations can be found using 188 a classical Mori-Zwanzig approach¹⁹, which is based on projecting the full dynamics on the slow variables and 189 general mathematical results provide evidence that deterministic, stochastic and non-Markovian components 190 should constitute the backbone of parameterizations^{17,178}. Recent studies show improvements over approaches 191 based on time-scale separation^{17,177,178}. 192

Recent studies have shown that stochastic approaches are also important for the prediction of extreme events and tipping points^{40,41,155,156}. Sura¹⁵⁶ discusses a stochastic theory of extreme events. He especially focuses on deviations from a Gaussian distribution; i.e. skewness and kurtosis, as first measures of extremes. He shows that multiplicative noise plays a significant role in causing non-Gaussian distributions. Franzke⁴⁰ shows that both deterministic nonlinearity and multiplicative noise are important in predicting of extreme events.

¹⁹⁸ 4 Statistical Physics Approaches to Stochastic Climate Theory

Significant progress has been achieved in the development of tractable and accurate statistical dynamical clo-199 sures for general inhomogeneous turbulent flows that are underpinned by exact stochastic models (see Box 2). 200 For an accessible review see the text book by Heinz⁵⁸. The statistical dynamical closure theory, pioneered by 201 Kraichnan⁷¹, has been recognized as a natural framework for a systematic approach to modelling turbulent 202 geophysical flows. Closure theories like the Direct Interaction Approximation (DIA),⁷¹ for homogeneous tur-203 bulence and the Quasi-Diagonal Direct Interaction Approximation (QDIA).⁴² for the interaction of mean flows 204 with inhomogeneous turbulence have exact generalized Langevin model representations⁶⁰. This means that 205 such closures are realizable; i.e. they have non-negative energy. 206

The first major application of turbulence closures has been the examination of the predictability of geo-207 physical flows. Early approaches applied homogeneous turbulence models to predicting error growth^{77,79,83} 208 whereas more recent advances by Frederiksen and O'Kane⁴⁶, O'Kane and Frederiksen¹¹³, building on the pi-209 oneering studies of Epstein³² and Pitcher¹³⁰, have enabled predictability studies of inhomogeneous strongly 210 non-Gaussian flows typical of the mid-latitude atmosphere. Turbulence closures have also been used for Subgrid-211 Scale Parameterisation (SSP) of the unresolved scales, for example eddies in atmospheric and ocean general 212 circulation models. Since it is generally only possible to represent the statistical effects of unresolved eddies 213 while their phase relationships with the resolved scales are lost ¹⁰⁰, statistical dynamical turbulence closures are 214 sufficient to allow SSPs to be formulated in a completely transparent way^{42,43,73,77,80,112,134}. Insights gained 215 through the development of inhomogeneous turbulence closure theory have motivated the recent development 216 of general stochastic forms for subgrid-scale parameterisations for geophysical flows⁶⁸. 217

²¹⁸ 4.1 Statistical dynamical closure theory

BOX 2 CLOSURE PROBLEM

In order to describe the statistical behavior of a turbulent flow the underlying nonlinear dynamical equations must be averaged. For simplicity we consider a generic equation of motion with quadratic nonlinearity for homogeneous turbulence, in which the mean field is zero, and the fluctuating part of the vorticity in Fourier space, $\hat{\zeta}_{\mathbf{k}}$, satisfies the equation:

$$\frac{\partial}{\partial t}\hat{\zeta}_{\mathbf{k}}(t) = K_{\mathbf{k}\mathbf{p}\mathbf{q}}\hat{\zeta}_{-\mathbf{p}}(t)\hat{\zeta}_{-\mathbf{q}}(t).$$
(3)

where **p** and **q** are the other wave numbers describing triad interactions i.e. $\mathbf{k} = (k_x, k_y)$ where $\delta(\mathbf{k} + \mathbf{p} + \mathbf{q}) = 1$ if $\mathbf{k} + \mathbf{p} + \mathbf{q} = 0$ and 0 otherwise. Here $K_{\mathbf{k}\mathbf{p}\mathbf{q}}$ are the interaction or mode coupling coefficients. The correlation between the eddies can now be represented by an equation for the covariance (cumulant in terms of wavenumbers \mathbf{k} and \mathbf{l}) which is found to depend on the third order cumulant in Fourier space:

$$\frac{\partial}{\partial t} \langle \hat{\zeta}_{\mathbf{k}}(t) \hat{\zeta}_{-1}(t') \rangle = K_{\mathbf{k}\mathbf{p}\mathbf{q}} \langle \hat{\zeta}_{-\mathbf{p}}(t) \hat{\zeta}_{-\mathbf{q}}(t) \hat{\zeta}_{-1}(t') \rangle.$$
(4)

Similarly the third order cumulant depends on the fourth order and so on such that we see that an infinite hierarchy of moment or cumulant equations is produced. Statistical turbulence theory is principally concerned with the methods by which this moment hierarchy is closed and the subsequent dynamics of the closure equations. The fact that for homogeneous turbulence the covariance matrix is diagonal greatly simplifies the problem. The majority of closure schemes are derived using perturbation expansions of the nonlinear terms in the primitive dynamical equations. The most successful theories use formal renormalization techniques^{19,58}.

The development of renormalized turbulence closures was pioneered by Kraichnan's Eulerian DIA⁷¹ for 220 homogeneous turbulence. The DIA, so named because it only takes into account directly interacting modes, 221 can be readily regularised to include approximations to the indirect interactions^{45,111} which are required to 222 obtain the correct inertial range scaling laws. Other homogeneous closures such as Herring's self consistent 223 field theory (SCFT⁵⁹) and McComb's local energy transfer theory (LET),⁹⁹ were independently developed soon 224 after. The DIA, SCFT and LET theories have since been shown to form a class of homogeneous closures that 225 differ only in whether and how a fluctuation dissipation theorem (FDT i.e. the linear response of a system to an 226 infinitesimal perturbation as it relaxes toward equilibrium) 15,25,44,71 is applied. As noted earlier, a consequence 227 of the DIA having an exact stochastic model representation is that it is physically realizable, ensuring positive 228 energy spectra. This is in contrast with closures based on the quasi-normal hypothesis which require further 229 modifications in order to ensure realizability; an example of such a closure is the eddy damped quasi-normal 230 Markovian (EDQNM) closure^{77,109,116} developed as a bets Markovian fit to the DIA. The EDQNM is dependent 231 on a choice of an eddy-damping parameter which can be tuned to match the phenomenology of the inertial 232 range. This Markovian assumption assumes that the rate at which the memory integral decays is significantly 233 faster than the time scale on which the covariances evolve. The relative success of these turbulence closures has 234 enabled the further study of the statistics of the predictability of homogeneous turbulent flows^{77-79,102}. 235

Frederiksen⁴² formulated a computationally tractable non-Markovian (memory effects) closure, the quasidiagonal direct interaction approximation (QDIA), for the interaction of general mean and fluctuating flow components with inhomogeneous turbulence and topography. The QDIA assumes that, prior to renormalisation, a perturbative expansion of the covariances are diagonal at zeroth order. In general, very good agreement has been found between the QDIA closure results and the statistics of DNS^{45,46,111}.

The non-Markovian closures discussed above are systems of integro-differential equations with potentially long time-history integrals posing considerable computational challenges, however various ways to overcome

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these challenges exist ^{44,46,111–115,135} and have been generalised to allow computationally tractable closure models for inhomogeneous turbulent flow over topography to be developed ^{42,46,111}. An alternative derivation of a stochastic model of the Navier-Stokes equations has been put forward by Memin ¹⁰⁷. It is based on a decomposition of the velocity fields into a differentiable drift and a stochastic component.

²⁴⁷ 4.2 Statistical dynamical and stochastic subgrid modelling

Many subgrid-scale stress models assume the small scales to be close to isotropic and in equilibrium such that 248 energy production and dissipation are in balance, similar to the eddy viscosity assumption of the Smagorinsky 249 model¹⁴⁸. Using the DIA, Kraichnan⁷¹ showed that for isotropic turbulence the inertial transfer of energy could 250 be represented as a combination of both an eddy viscous (on average energy drain from retained to subgrid 251 scales) and stochastic back-scatter (positive semi-definite energy input from subgrid to retained scales) terms. 252 The nonlinear transfer terms represented by eddy viscosity and stochastic back-scatter are the subgrid processes 253 associated with the respective eddy-damping and nonlinear noise terms that constitute the right hand side of 254 the DIA tendency equation for the two-point cumulant $\frac{\partial}{\partial t} \langle \hat{\zeta}_{\mathbf{k}}(t) \hat{\zeta}_{-\mathbf{k}}(t') \rangle$. Leith⁷⁷ used the EDQNM closure to 255 calculate an eddy dissipation function that would preserve a stationary k^{-3} kinetic energy spectrum for two-256 dimensional turbulence. Kraichnan⁷³ developed the theory of eddy viscosity in two and three dimensions and 257 was the first to identify the existence of a strong cusp in the spectral eddy viscosity near the cutoff wavenumber 258 representing local interactions between modes below and near the cusp. Rose¹³⁴ argued for the importance of 259 eddy noise in subgrid modelling. 260

O'Kane and Frederiksen¹¹² calculated QDIA based SSPs considering observed atmospheric flows over global topography and quantifying the relative importance of the subgrid-scale eddy-topographic, eddy-mean field, quadratic mean and mean field-topographic terms. They also compared the QDIA based SSPs to heuristic approaches based on maximum entropy, used to improve systematic deficiencies in ocean climate models⁶². While closure models may be the natural starting place for developing subgrid-scale parameterisations, their complexity makes them difficult to formulate and apply to multi-field models like GCMs, even though successful studies exist^{68,180}.

²⁶⁸ 5 Stochastic Parametrisation Schemes in Comprehensive Models

Climate and weather predictions are only feasible because the governing equations of motion and thermody-269 namics are known. To solve these equations we need to resort to numerical simulations that discretize the 270 continuous equations onto a finite grid and parameterize all processes that cannot be explicitly resolved. Such 271 models can be characterized in terms of their dynamical core, which describe the resolved scales of motion, and 272 the physical parameterizations, which provide estimates of the grid-scale effect of processes which cannot be 273 resolved by the dynamical core. This general approach has been hugely successful in that nowadays predictions 274 of weather and climate are made routinely. On the other hand, exactly through these predictions it has become 275 apparent that uncertainty estimates produced by current state-of the art models still have shortcomings. 276

One shortcoming is that many physical parameterizations are based on bulk formula which are based on the assumption that the subgrid-scale state is in equilibrium with the resolved state¹¹⁸. Model errors might arise from a misrepresentation of unresolved subgrid-scale processes which can affect not only the variability, but also the mean error of a model^{129,141}. An example in a comprehensive climate model is e.g., the bias in the 500hPa geopotential height pattern, which is reduced when the representation of the subgrid-state is refined⁷ (Fig. 2).

In recent years, methods for the estimation of flow-dependent uncertainty in predictions have become an important topic. Ideally, uncertainties should be estimated within the physical parameterizations and uncertainty representations should be developed alongside the model. Many of these methods are "ad hoc" and added *a posteriori* to an already tuned model. Only first steps to develop uncertainty estimates from within the parameterizations have been attempted^{20,131}.

The representation of model-error in weather and climate models falls in one of two major categories: 287 Multi-model approaches and stochastic parameterizations. In the multi-model approach each ensemble mem-288 ber consists of an altogether different model. The models can differ in the dynamical core and the physical 289 parameterizations^{55,63,75} or use the same dynamical core but utilize either different static parameters in their 290 physical parameterizations¹⁵¹ or altogether different physics packages^{6,31,106,152}. Both approaches have been 291 successful in improving predictions of weather and climate over a range of scales, as well as their uncertainty. 292 Multi-model ensembles provide more reliable seasonal forecasts 122 and are commonly used for the uncertainty 293 assessment of climate change predictions e.g., as in the Assessment Report 5 of the Intergovernmental Panel 294 on Climate Change (IPCC)¹⁵⁷. Stochastic parameterizations are routinely used to improve the reliability of 295 weather forecasts in the short- 6 and medium-range 5,10,123 as well as for seasonal predictions 4,28,165 . 296

In the stochastic approach, the effect of uncertainties due to the finite truncation of the model are treated 297 as independent realizations of stochastic processes that describe these truncation uncertainties. This treatment 298 goes back to the idea of stochastic-dynamic prediction^{33,118,130}. While the verdict is still open if subgrid-scale 299 fluctuations must be included explicitly via a stochastic term, or if it is sufficient to include their mean influence 300 by improved deterministic physics parameterizations, one advantage of stochastically perturbed models is that all 301 ensemble members have the same climatology and model bias; while for multi-parameter, multi-parameterization 302 and multi-model ensembles each ensemble member is *de facto* a different model with its own dynamical attractor. 303 For operational centers the maintenance of different parameterizations requires additional resources and due to 304 the different biases makes post-processing very difficult. 305

³⁰⁶ 5.1 Stochastic Parameterizations in Numerical Weather Prediction

Due to the chaotic nature of the dynamical equations governing the evolution of weather, forecasts are sensitive 307 to the initial condition limiting the intrinsic predictability of the weather system^{82,84}. Probabilistic forecasts 308 are performed by running ensemble systems, where each member is initialized from a different initial state and 309 much effort has gone into the optimal initialization of such ensemble systems^{63,108,161}. Nevertheless state-of-310 the-art numerical weather predictions systems continue to produce unreliable and over-confident forecasts¹⁴. 311 Consequently, the other source of forecast uncertainty - model-error - has received increasing attention^{117,118}. 312 Since for chaotic systems model-error and initial condition error will both result in trajectories that will diverge 313 from the truth, it is very difficult to disentangle them 149 . 314

The first stochastic parameterization used in an operational numerical weather prediction model was the 315 stochastically perturbed physics tendency scheme (SPPT), sometimes also referred to as stochastic diabatic 316 tendency or Buizza-Miller-Palmer (BMP) scheme¹³. SPPT is based on the notion that – especially as the 317 horizontal resolution increases – the equilibrium assumption no longer holds and the subgrid-scale state should 318 be sampled rather than represented by the equilibrium mean. Consequently, SPPT multiplies the accumulated 319 physical tendencies of temperature, wind and moisture at each grid-point and time step with a random pattern 320 that has spatial and temporal correlations. In other words, SPPT assumes that parameterization uncertainty can 321 be expressed as a multiplicative noise term. Ensemble systems perturbed with the SPPT scheme show increased 322 probabilistic skill mostly due to increased spread in short and medium-range ensemble forecasts^{8,13,132,159}. 323

A second successful stochastic parameterization scheme, is the so-called stochastic kinetic energy-backscatter 324 scheme (SKEBS) whose origin lies in Large-Eddy Simulation modeling⁹⁸ and has recently been extended to 325 weather and climate scales^{142,143}. The key idea is that energy associated with subgrid processes is injected 326 back onto the grid using a stochastic pattern generator. This method has been successfully used in a number 327 of operational and research forecasts across a range of scales^{5,6,8,10,11,16,138}. Similar to the SPPT scheme, 328 ensemble systems with SKEBS increase probabilistic skill by increasing spread and decreasing the root-mean-329 square (RMS) error of the ensemble mean forecast. First results of these schemes at a convection-permitting 330 resolution of around 4km report also a positive impact on forecast skill, in particular more reliable precipitation 331 forecasts 12,133 . 332

³³³ 5.2 Stochastic Parameterizations in Climate Models

The use of stochastic parameterization in climate models is still in its infancy. Climate prediction uncertainty assessments, e.g., IPCC¹⁵⁰, are almost exclusively based on multi-models, mostly from different research centers. Part of the problem is that on climate timescales, limited data for verification exists. A second reason is that on longer timescales, bias is a major source of uncertainty and traditional multi-models are very efficient at sampling biases, although such an experiment is poorly designed for an objective and reliable uncertainty assessment.

However, in recent years first studies have emerged which demonstrate the ability of stochastic parame-330 terizations to reduce longstanding biases and improve climate variability (see Fig. 2 for an example). Jin 340 and Neelin⁸¹ developed a stochastic convective parameterization that includes a random contribution to the 341 convective available potential energy (CAPE) in the deep convective scheme. They find that adding convective 342 noise results in enhanced eastward propagating, low-wavenumber low-frequency variability. Berner et al.⁷ in-343 vestigate the impact of SKEBS on systematic model-error and report an improvement in the representation of 344 convectively-coupled waves leading to a reduction in the tropical precipitation bias. Furthermore, Majda and 345 colleagues developed systematic stochastic multi-cloud parameterizations for organized convection^{47,67,94,95}. 346 The multi-cloud approach is based on the assumption that organized convection involves three types of clouds 347 and the evolution from one cloud type to another can be described by a transition matrix. 348

A longstanding systematic error of climate models is the underestimation of the occurrence of Northern 349 Hemispheric blocking. Stochastic parameterizations have been demonstrated to be one way to increase their 350 frequency 4,28,53,165 , although, e.g. increasing horizontal resolution, leads to similar improvements 7,24 . This 351 suggests that while it might be necessary to include subgrid-scale variability in some form, the details of this 352 representation might not matter. On the other side, Berner et al.⁷ argue that this degeneracy of response 353 to different subgrid-scale forcings warrants a cautionary note: namely that a decrease in systematic error 354 might not necessarily occur for the right dynamical reasons. The opposite holds true, as well: Due to the 355 necessary tuning of parameters in the parameterizations of comprehensive climate models, an improvement 356 in the formulation of a physical process might not immediately lead to an improved model performance. A 357 striking example of compensating model errors is described in Palmer and Weisheimer¹¹⁹, who report how an 358 inadequate representation of horizontal baroclinic fluxes resulted in a model error that was equal and opposite to 359 the systematic error caused by insufficiently represented vertical orographic gravity wave fluxes. Improvements 360 to wave drag parameterization without increasing resolution unbalanced the compensating model errors, leading 361 to an increase in systematic model bias. 362

Williams¹⁷⁵ studied the effect of including a stochastic term in the fluxes between the atmospheric and oceanic components in a coupled ocean-atmosphere model. He reports changes to the time-mean climate and increased variability of the El Nino Southern Oscillation, suggesting that the lack of representing of sub-grid variability in air-sea fluxes may contribute to some of the biases exhibited by contemporary climate models.

On seasonal timescales where sufficient observational data for a probabilistic verification exist, stochastic parameterizations have been reported to increase predictive skill. For example, ensemble forecasts of the sea surface temperatures over the Nino3.4 region showed increased anomaly correlation, decreased bias and decreased root mean square error in coupled ocean-atmosphere models^{4,28,165}.

371 6 Conclusion

We postulate the use of stochastic-dynamical models for uncertainty assessment and model-error representation in comprehensive Earth-System models. This need arises since even state-of-the-art weather and climate models cannot resolve all necessary processes and scales. Here we reviewed mathematical methods for stochastic climate modeling as well as stochastic subgrid-scale parameterizations and postulate their use for a more systematic strategy of parameterizing unresolved and unrepresented processes.

In the last decade, a number of studies emerged that demonstrate the potential of this approach, albeit

applied in an ad hoc manner and tuned to specific applications. Stochastic parameterizations have been shown
to provide more skillful weather forecasts than traditional ensemble prediction methods, at least on timescales
where verification data exists. In addition, they have been shown to reduce longstanding climate biases, which
play an important role especially for climate and climate change predictions.

Here we argue, that rather than pushing out the limit of skillful ensemble predictions by a few days, more attention should be given on the assessment of uncertainty (as already proposed, e.g., Smith¹⁴⁹). Ideally, it should be carried out alongside the physical parameterization and dynamical core development and not added *a posteriori*. The uncertainty should be directly estimated from within the parameterization schemes and not tuned to yield a particular model performance, as is current practice. For example, Sapsis and Majda¹³⁹,¹⁴⁰ propose a statistical framework which systematically quantifies uncertainties in a stochastic fashion.

The fact that according to the last two assessment reports (AR) of the IPCC (AR4¹⁴⁷ and AR5¹⁵⁰) the uncertainty in climate predictions and projections has not decreased may be a sign that we might be reaching the limit of climate predictability, which is the result of the intrinsically nonlinear character of the climate system (as first suggested by Lorenz⁸²).

Recently Palmer¹²¹ argued that due to limited computational and energy power resources, predictable scales 392 should be solved accurately, while the unpredictable scales could be represented inaccurately. This strategy is at 303 the core of the systematic mode reduction reviewed here, but has only recently been considered for comprehensive 394 Earth-System Models. Stochastic models focus on the accurate simulation of the large, predictable, scales, while 395 only the statistical properties of the small, unpredictable, scales are captured. This has been demonstrated, 396 e.g, by Franzke and Majda³⁸, Kravtsov et al.⁷⁴, who successfully applied mode reduction strategies to global 397 atmospheric circulation models. They showed that these reduced models consisting of only 10-15 degrees of 398 freedom reproduced many of the important statistics of the numerical circulation models which contained a few 399 hundreds degrees of freedom. Vanden-Eijnden¹⁶³ proposed numerical approaches for multi-scale systems where 400 only the largest scales are explicitly computed and the smaller scales are approximated on the fly. 401

The recent result of Wouters and Lucarini^{177,178} provide a promising path towards a general theory of parametrizations for weather and climate models, and give theoretical support that parameterization schemes should include deterministic, stochastic and non-Markovian (memory) components. Moreover, Wouters and Lucarini's results suggest that there is common ground in developing parameterizations for weather and climate prediction models. Optimal representations of the reduced dynamics based on Ruelle's response theory and the Mori-Zwanzig formalism coincide, thus, providing equal optimal representations of the long-term statistical properties and the finite-time evolution of the slow variables.

One exciting future research area is the use of stochastic methods for use in data assimilation, which is already an active field of research ^{51,54,65,104,114,115,133}. Stochastic methods have been shown to increase the ensemble spread in data assimilation, leading to a better match between observations and model forecasts ^{54,105,133}. A cutting-edge frontier is the use of order moments and memory effects in Kalman filter data assimilation schemes¹¹⁵. Another emerging field is the use of stochastic parameterizations in large climate ensembles, which would allow the comparison of uncertainty estimates based in multi-models to that of stochastically perturbed ones.

⁴¹⁶ Our hope is that basing stochastic-dynamic prediction on sound mathematical and statistical physics con-⁴¹⁷ cepts will lead to substantial improvements, not only in our ability to accurately simulate weather and climate, ⁴¹⁸ but even more importantly to give proper estimates on the uncertainty of these predictions.

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Figure 1: Regime transitions in a rotating two-layer annulus laboratory experiment, viewed from above. Different colours correspond to different internal interface heights, through the use of a sophisticated visualisation technique¹⁷⁰. In the upper row, small-scale inertia–gravity waves are absent, and large-scale regime transitions do not occur. In the lower row, small-scale inertia–gravity waves are present locally in the troughs of the large-scale wave, and a large-scale regime transition does occur. From the laboratory experiments of Williams et al.^{168,169,172,173}.



Figure 2: Mean systematic error of 500 hPa geopotential height fields (shading) for extended boreal winters (December–March) of the period 1962-2005. Errors are defined with regard to the observed mean field (contours), consisting of a combination of ERA-40 (1962-2001) and operational ECMWF analyses (2002-2005). (a) Systematic error in a numerical simulation with the ECMWF model IFS, version CY32R1, run at a horizontal resolution of T_L95 (about 210km) and 91 vertical levels. (b) Systematic error in a simulation with a stochastic kinetic-energy backscatter scheme (SKEBS). Significant differences at the 95% confidence level based on a Student's t-test are hatched. After Berner et al.⁷.