On defining climate by means of an ensemble

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Abstract

We study the suitability of an initial condition ensemble to form the conceptual basis of defining climate. We point out that the most important criterion is the uniqueness of the probability measure on which the definition relies. We first propose, in harmony with earlier work, to represent such a probability measure by the distribution of ensemble members that have converged to the probability density of the natural probability measure of the so-called snapshot or pullback attractor of the dynamics, which is time dependent in the presence of external forcing. Then we refine the proposal by taking a density that is conditional on the (possibly time-evolving) state of system components with time scales longer than the horizon of a particular study. We discuss the applicability of such a definition in the Earth system and its realistic models, and conclude that micro initialization from observations in slower system components perhaps provides the practically relevant probability density after a few decades of convergence. However, the absence of sufficient time scale separation between system components or regime transitions in slower system components might preclude uniqueness, at least in certain subsystems, and time evolution in slower system components might induce unforced climate changes, leading to the need for targeted investigations to determine the forced response. We propose an initialization scheme for studying all these issues in Earth system models.
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ABSTRACT: We study the suitability of an initial condition ensemble to form the conceptual basis of defining climate. We point out that the most important criterion is the uniqueness of the probability measure on which the definition relies. We first propose, in harmony with earlier work, to represent such a probability measure by the distribution of ensemble members that have converged to the probability density of the natural probability measure of the so-called snapshot or pullback attractor of the dynamics, which is time dependent in the presence of external forcing. Then we refine the proposal by taking a density that is conditional on the (possibly time-evolving) state of system components with time scales longer than the horizon of a particular study. We discuss the applicability of such a definition in the Earth system and its realistic models, and conclude that micro initialization from observations in slower system components perhaps provides the practically relevant probability density after a few decades of convergence. However, the absence of sufficient time scale separation between system components or regime transitions in slower system components might preclude uniqueness, at least in certain subsystems, and time evolution in slower system components might induce unforced climate changes, leading to the need for targeted investigations to determine the forced response. We propose an initialization scheme for studying all these issues in Earth system models.
SIGNIFICANCE STATEMENT: The laws of nature permit a range of states of the climate system at any time; weather is generated as they follow each other. An increasingly popular approach is to try to represent these states by an ensemble of climate model simulations. Our aim is a careful exploration of implications of fundamental theoretical considerations regarding such a representation. We argue that the distribution of ensemble members needs to be conditioned on the state of slower system components (e.g., the deep ocean) in century-scale studies. We point out that the uniqueness of this distribution must be verified in such cases, for which we propose an initialization scheme, and that unforced climate changes might be possible during variations in slower system components.

1. Motivation and historical background

In the past decade, $O(10)–O(100)$-member initial-condition ensemble simulations in single state-of-the-art Earth system models have been run (e.g., Kay et al. 2015; Maher et al. 2019), and such simulations are expected to become widespread in the near future. The aim of these projects is the identification of forced responses and the exploration of the internal variability of climate under explicit time dependence (which the word ‘forcing’ will refer to throughout this article). The motivation for this kind of investigation is based on the naive recognition (e.g., Deser et al. 2020, and references therein) that the Earth system (and models thereof) permits a plethora of equally plausible states (e.g., weather configurations) at any time instant of a forcing scenario: the ensembles in question are intended to represent this set of states of the system, for which their different members have been generated with the same forcing scenario but from different initial conditions. Climatological mean values are then identified with the ensemble mean, and the internal variability of climate is (or at least should be) described by further statistical quantifiers evaluated with respect to the ensemble; and the time evolution of all these statistical quantifiers (including but not restricted to the mean) is identified with their forced response.

One assumption behind these interpretations is that climate is defined through the distribution of the ensemble members. However, in case this distribution is not unique but depends on personal choices (e.g., on the time and way of initialization), every research group creating an ensemble simulation may happen to define its own climate even using the same model and forcing scenario: such a climate is not characteristic to the system and the forcing scenario alone (i.e., the ensemble
members do not trace out an unconditional *a priori* (Paillard 2008) probability distribution in this sense), so that, due to the dependence on the aforementioned personal choices, it is a “personal climate”, which should be avoided (cf. Werndl 2019). An aim of this article is a deeper investigation of this issue.

Traditionally, specific definitions of climate, beyond identifying it with a statistical description of the “climate system” or the Earth system, were usually formulated in terms of *temporal* statistics of weather (e.g., Stocker et al. 2013), a practice that is still well and alive (Nicklas et al. 2022). If no forcing acted on the Earth system, i.e., if its equations of motion (including boundary conditions) did not depend explicitly on time, the interval for evaluating temporal statistics could be extended to the infinite future, and these statistics would coincide with those evaluated with respect to an infinite-size ensemble distributed according to the natural probability measure of the chaotic attractor of the system (Ott 1993) (i.e., Birkhoff’s ergodic theorem would hold; note that the Earth system is dissipative, and is generally assumed to be chaotic). The same would be true for a temporally periodic forcing handled in terms of a stroboscopic map (Tél and Gruiz 2006). However, if the forcing is not periodic, such a construction is not available. In that case, statistical quantifiers evaluated with respect to time need not correspond to any probability measure that would be relevant for any particular time instant (Drótos et al. 2015) (this is most easily seen if the system is forced by a monotonic drift).

While Lorenz recognized the phenomenon (namely chaos) that renders the evolution of the state of the system unpredictable (Lorenz 1963), and also formulated that the permitted states of the system may be represented by an ensemble of realizations that differ in their initial conditions (Lorenz 1975), his notion of climate still assumed that the statistical descriptors are approximately constant for shorter or longer times (Lorenz 1975). At the same time, Hasselmann (1976) was thinking about a statistical mechanical analogy that implied the relevance of an ensemble but without justification. Leith (1975a,b, 1978) worked out the same statistical mechanical analogy in more detail and including the change of the ensemble statistics as a response to some external forcing (but assuming slow variation of the latter). He was explicitly motivated by the unpredictability of the individual realizations, but he did not discuss how the distribution of the ensemble members is determined and if it is unique.
Branstator and Teng (2010) revived the latter picture, allowed for variations in the forcing on any time scale, and also assumed (but not justified) the uniqueness of a distribution, already called *climatological* distribution, emerging from arbitrary initial conditions in the infinite past. This climatological distribution gave the reference for ensembles of trajectories (or abstract probability densities) initialized later, by which predictability was studied. Finally, DelSole and Tippett (2018) adopted their approach, discussed uniqueness in dynamical systems, and demonstrated it in a stochastic model, providing thereby with a well-established notion of the “standard” climatological distribution. Also interested in predictability, however, they were not satisfied with this notion, and introduced a precise probabilistic framework that based a climatological distribution on observations of the more recent past. By such a definition, the unconditional nature of the concept of climate (a unique distribution in a given system subject to a given forcing) is again lost. (Note that loss of predictability and convergence to a unique distribution are two facets of the same phenomenon: climate should be identified when predictability is lost.)

Actually, Ghil et al. (2008) already drew attention to the climatological relevance of uniqueness of probability distributions in nonautonomous systems, and claimed on a mathematical basis that a probability density converges to a unique one at a given time $t$ if its initialization time $t_0$ tends to $-\infty$ in a dissipative chaotic system. In particular, this unique density corresponded to the natural probability measure of a so-called pullback attractor, and was shown to be traced out by an ensemble of trajectories initialized in the remote past. However, Ghil et al. (2008) and related work (e.g., Chekroun et al. 2011; Ghil 2014; Pierini et al. 01 Jun. 2016) applied this concept to subsystems of the Earth, which were subject to randomly generated forcing with a fixed distribution instead of a drifting signal. Even the review by Ghil and Lucarini (2020) hardly mentions the latter possibility. Although Werndl (2016) applied the concept of pullback attractors to general forms of forcing, including drifting ones, she discarded the corresponding definition of climate.

In fact, it was in Bódai and Tél (2012) that the applicability of the approach of Ghil et al. (2008) to the description of global climate changes was first recognized by writing that “climate change can be seen as the evolution of snapshot attractors” (and note that the correspondence between the rigorously defined pullback attractor and the so-called snapshot attractor, which was introduced to the physics literature by Romeiras et al. (1990), was pointed out there). We discussed in detail in Drótos et al. (2015) that the uniqueness of the natural probability measure of a pullback or
snapshot attractor (as represented by an initial-condition ensemble, although in a toy model) makes it the appropriate concept for describing the statistics, i.e., the climate, of a system forced by a drifting signal (both in terms of the “mean state” and in that of the internal variability, both of which respond to a forcing). In Herein et al. (2016) the applicability of this framework to an intermediate-complexity general circulation model was illustrated, which was also used in Herein et al. (2017) to extend the framework to variables describing spatial patterns. In Drótos et al. (2017) we also pointed out the practical relevance of the approach in the same model by investigating the convergence to the density of the natural probability measure from initial conditions obtained by a slight perturbation of a state of the system already located on the attractor. The conceptual power of the snapshot/pullback framework was underlined by Vincze et al. (2017) by applying it to a laboratory experiment. An overview of basics and applications of this framework to describe climate is provided in Tél et al. (2020), where previously disregarded issues are also discussed.

In this article, it is explained why the description based on the natural probability measure of an attractor could actually be regarded as a natural definition of climate, and, through a thorough analysis, why this definition or an improved version thereof might still prove to be imperfect for a practical description of the statistics of the real Earth system and its fully coupled models. In that case, it may still serve as a guidance for how to theoretically treat probabilistic aspects and how to design practically useful constructions.

A closer look at the concept of forced response will also be taken, highlighting that a climate conditioned on the initial state of slow system components can change without the introduction of a forcing.

2. A first proposal for the definition of climate

Let us imagine that the dynamics of the Earth system is described perfectly (even including the discretized nature of the model) by the intermediate-complexity model Planet Simulator (PlaSim) (Fraedrich et al. 2005) with a mixed-layer ocean [in the configuration used in Drótos et al. (2017)]. This defines our dynamical system, which has a phase space of \( \approx 10^5 \) variables. Let our model
Fig. 1. The annual mean near-surface temperature $T$ of a single grid point in the southern Pacific Ocean (at $180^\circ$E and about $64^\circ$S) as a function of time. $t_0 = 610$ yr is identified with the present, and $t_1 = 694$ yr is an arbitrarily chosen year in the future. The dark gray line is a single PlaSim simulation and is regarded as the instrumental record in the model system. The red line is the continuation of the same simulation and is regarded as a prediction. The 48 light blue lines are alternative predictions, obtained from simulations initialized by slightly perturbing the surface pressure field of the simulation of the dark gray line at $t_0 = 610$ yr [see the main text and Drótos et al. (2017) for details]. The normalized histogram $h_T$ constructed from the 48 values of the light blue lines and further 144 alternative predictions (a total of 192 values) at $t_1$ is shown on the right-hand-side of the main plot. The CO$_2$ concentration, through which the forcing scenario is defined, is also displayed (in orange). The vertical dot-dashed line in gray marks the beginning of the linear ramp in the CO$_2$ concentration. Data are from Drotos (2022).

Earth system be subject to the following forcing scenario:

$$[\text{CO}_2](t) = \begin{cases} 
360 & \text{for } t < 600, \\
360 + 3.6(t - 600) & \text{for } t \geq 600,
\end{cases}$$

where concentration is in ppm and time is in yr, and let us study the time evolution of the annual mean near-surface temperature in a particular grid point in the southern Pacific [similarly as in Drótos et al. (2017)]. Finally, let us suppose that our Earth system has followed the trajectory corresponding to the dark gray line of Fig. 1 up to $t_0 = 610$ yr, which we identify with the present.
A possible question about the weather of the future is the near-surface temperature of the given grid point at $t_1 = 694$ yr. To obtain this, we can use the $t = t_0$ phase space position of the dark gray trajectory of Fig. 1 as initial condition, and integrate PlaSim from $t_0$ to $t_1$: the result for the near-surface temperature of the given grid point is the red trajectory shown in Fig. 1, which has, of course, a unique value in $t_1$. However, this value is only one possible answer to the question.

Let us slightly perturb the $t = t_0$ phase space position of the dark gray trajectory 192 times to obtain 192 different initial conditions: the utilized random perturbation modifies the surface pressure field on the order of $10^{-3}$ hPa [see again Drótos et al. (2017) for the details], so that each perturbed initial condition can be regarded as realistic as the original one. In particular, these different initial conditions could not be distinguished by standard instrumental measurements on the real Earth. The integration of PlaSim from these initial conditions results in an ensemble of trajectories, plotted in light blue in Fig. 1 (only 48 of the 192 for better visibility), each giving a separate answer for the weather in $t_1$. All are possible answers, and the differences between them emerge as a result of the chaotic nature (internal variability, unpredictability) of the system.

In fact, infinitely many of these answers would trace out a density, as indicated by the normalized histogram $h_T$ in Fig. 1. We can ask now if this density provides a relevant characterization of the plethora of all possible near-surface temperature values in $t_1$.

In particular, the question is about the uniqueness of this density. If we perturb the original initial condition in $t_0$ in a different way, will we end up with a different density in $t_1$? For example, if we take a larger or a smaller magnitude for the perturbation, will the final density be broader or more narrow? Or if we restrict the sign in the perturbation, will it shift the final density in some direction?

In fact, for an infinitely large ensemble in a dissipative nonautonomous dynamical system exhibiting chaotic behavior (like PlaSim), the density in question corresponds to the natural probability measure of a snapshot (Romeiras et al. 1990) or pullback (Ghil et al. 2008; Chekroun et al. 2011) attractor if $t_0$ tends to $-\infty$, at least as long as the initial conditions remain in the basin of attraction of the same attractor (provided that the relevant basin of attraction existed in the infinitely remote past, cf. Section 3). This implies that the probability density in question is unique, i.e., it will be the same for practically any set of infinitely numerous initial conditions within the basin of attraction of the given attractor. In Drótos et al. (2015), an atmospherically motivated toy model was used
Fig. 2. The light blue lines and histogram of Fig. 1 compared to an ensemble of the same size (marked by dark gray) initialized in the remote past (at $t = 0$, asymptotically far in practice from $t = 575$). The corresponding ensemble averages are also shown in dark blue and green, respectively. By $t^*$, the two ensemble averages practically coincide. Data are from Drotos (2022).

to illustrate that the process of convergence to the natural probability measure is exponential-like on the long term (it is presumably faster than any power law, cf. Appendix 5). In such a case, the convergence of a finite-size ensemble is practically accomplished (with “exponential precision”, according to some practical point of view) within a finite amount of time (so that tending to $-\infty$ with $t_0$ is not required). In Herein et al. (2016), this was found to be the case for PlaSim, too, and this finding was conjectured to be relevant for any global climate model or Earth system model. In our configuration of PlaSim, the convergence time proved to be a few decades.

As a consequence, the probability density of the near-surface temperature in the investigated grid point in our configuration (and that of any other variable or set of variables in similar systems) that is traced out by even a finite-size ensemble at $t_1$ will be practically the same regardless of how we choose initial conditions in $t_0$ — provided that two conditions are met. The first is that $t_0$ has to be sufficiently far, although not infinitely far, in the past from $t_1$. The second is that the initial conditions must be chosen within such limits that ensure convergence to the desired attractor, avoiding a different one, e.g. a snowball Earth (cf. Kaszás et al. 2019; Ragon et al. 2022). Since $t_0$ and $t_1$ are separated by several decades in Fig. 1, this conclusion translates for our example as follows: within the mentioned limits, we cannot modify the initialization scheme in $t_0$ to obtain a substantially different probability density in $t_1$; that is, within a certain range of initialization
schemes, we cannot “ruin” the quantitative result. Among other initialization schemes (which need not rely on some particular trajectory of the system), an extremely small perturbation of the actually realized initial conditions (the $t = t_0$ phase space position corresponding to the dark gray line of Fig. 1 in our model Earth system, the equivalent of hypothetical perfect instrumental observations at $t_0$ in the real Earth system) will lead to this unique density, which corresponds to the natural probability measure, see Fig. 2.

These considerations suggest this unique density (the ‘natural probability density’ in what follows) to be the practically relevant $a$ $priori$ (Paillard 2008) probability density (i.e., existing independently of any observation about the system) that can be associated with the plethora of all possibilities in $t_1$ that are permitted by the dynamics under the given forcing history (and within the relevant basin of attraction). That is, beyond being of practical interest, the natural probability density characterizes the system in statistical or probabilistic terms, instead of characterizing a particular situation (a “microstate” in a statistical mechanical analogy, e.g., a weather configuration in the atmosphere) permitted by the system. Note that this abstract density exists at any time instant: not only at $t_1$, but also after and even before it (for instance, also at $t_0$, or even earlier; see the dark gray ensemble of Fig. 2). To practically obtain this density at a given time instant, one just has to prescribe initial conditions for an ensemble in the sufficiently far past (within the relevant basin of attraction), and follow the time evolution of the ensemble until the desired time instant. Of course, the natural probability density depends on time in the presence of a forcing (which is the generic situation and is so in the dynamics of the real Earth system; see again the dark gray ensemble of Fig. 2 for our model configuration). Otherwise, it is constant, and coincides with the natural probability density of the usual chaotic (stationary) attractor of the dynamical system (Ott 1993).

Note that the natural probability density should actually be defined in the full phase space of the system. The probability density of a given variable (like the near-surface temperature of the selected grid point in the example of Figs. 1-2) is the marginal density of this multivariate probability density. The full multivariate probability density carries information about the statistical relationships between different parts of the system (different variables, different geographical regions, etc.); in other words, about the structure of internal variability.
As a subtlety, the natural probability measure is defined instantaneously in mathematical terms, whereas our numerical example considered an annual mean. This apparent discrepancy is easy to resolve. On the one hand, the individual time evolution of the trajectories composing the ensemble results in their phase space positions to be distributed according to the natural probability density at any time instant; on the other hand, since a particular solution of a dynamical system is unique, the time evolution of the trajectories also uniquely defines a probability density for temporal averages evaluated along these individual trajectories. (In fact, this is true not only for averages, but for any quantity derived from an interval of time or simply from more than one discrete time instant.) The latter construction was termed “interval-wise taken” in Drótos et al. (2015). For the annual mean near-surface temperature of our example, this density is what we called the natural probability density. We thus see that generalization to some finite time interval of interest (days, months, years, etc.) is straightforward.

We recall now that any definition of climate intends to capture statistical properties. We also see that the relevant statistical properties of the system are, at the root, described by the natural probability measure of the relevant snapshot or pullback attractor at any time instant. Therefore, we would hereby suggest defining climate as the statistical properties as determined by the (infinitely large) ensemble of trajectories evolving according to the natural probability measure under a given forcing history. Then the expected value of some given variable will be the climatic mean value of that variable, and all higher-order moments will describe internal variability. With this definition, any particular realization of the dynamics performs a sampling of the probability density that defines climate [i.e., the ‘climatological distribution’ in the terminology of Branstator and Teng (2010)].

3. Applicability in modeling; a conditional definition

In practical numerical modeling, the natural probability density is approximately represented by the distribution of a finite-size ensemble. Although we based our considerations for constructing the definition on the numerical example of our PlaSim configuration, any global climate model or Earth system model shares the most relevant properties: they are nonautonomous dissipative dynamical systems. Due to discretization, they have a finite number of variables, but, on the one hand, it is plausible to think that a system described by partial differential equations should
be obtained as a limit of infinitely many ordinary differential equations and thus exhibits similar behavior; and, on the other hand, spatial autocorrelation reduces the effective number of degrees of freedom to a finite value. As a consequence, our considerations can presumably be extended both to other models and to the real Earth system.

From the point of view of numerical modeling, however, the nonzero difference between the light blue ensemble and the natural probability density (represented by the dark gray ensemble) approximately up to $t^* = 650$ in Fig. 2 implies a warning: before convergence to the natural probability density takes place up to some practically prescribed accuracy, a numerical ensemble of trajectories does not represent the statistical properties relevant for climate according to the criteria discussed above (Drótos et al. 2017). Climate-related studies should, in principle, utilize ensembles for which such a convergence has taken place. (With a term frequently used by the modeling community, the ‘ensemble spread’ must already correctly describe the natural probability density with some accuracy imposed by some practical aspect.)

Unfortunately, the practical situation may be unfavorable from this point of view: the issue of nonzero convergence time poses a conceptual problem if the evolution of some variables of the system are characterized by long time scales (implying long convergence times) relative to the horizon of a particular study. As a prominent example in the real Earth system and in fully coupled models thereof, time scales up to the order of 1000 years may appear in the deep ocean (Li and Jarvis 2009), while studies with immediate practical relevance concentrate on the last and forthcoming few centuries. (For the theoretical background of identifying different time scales, see Appendix 5.)

In such a situation, one would presumably not wish to take the full variability introduced by these slow processes into account. In the ideal case of an infinitely large separation between the long and the targeted time scales, one might utilize a single realization (actually, a single value, a single “microstate”) in the variables associated with the long time scales (‘slow variables’ in what follows), e.g. based on instrumental observations [cf. DelSole and Tippett (2018) and the corresponding discussion below]. Utilizing a single realization would lead to a conditional probability measure for the rest of the system, and a corresponding conditional definition of climate. This would be the natural probability measure of the subsystem obtained by fixing the values of the slow variables and would thus be unique (within a given basin of attraction).
In case of a finite but large separation between the time scales, the conditional definition should follow some time evolution in the slow variables, which could also induce some time dependence in the “natural measure” defined over the faster variables, provided that such an approximately unique “natural measure” can be found and persists. A generalization of the theory of slow-fast systems (Kuehn 2015) to nonautonomous dynamics might help construct a precise definition of a conditional “natural measure”. However, if the separation is not sufficiently large, it might not be possible to define a conditional probability measure that would be unique in the faster variables, neither mathematically nor in practice.

DelSole and Tippett (2018) recognize the problem of possibly unseparated time scales and suggest to resolve it by conditioning the definition of climate on observations of the past. However, such a definition may not be satisfactory, since it involves two kinds of ambiguity. First, such a climate depends (practically continuously) on how far in the past the observations (more precisely, initial conditions compatible with the observations) are prescribed: if the lead time may be chosen on a case-by-case basis, we will end up at the concept of “personal climate” discussed in the Introduction, and there will be no qualitative difference between the notion of climate and that of probabilistic weather forecast. Second, such a climate will depend on the precision of observations: improving precision may narrow down the magnitude of internal variability.

These undesired dependences will generally disappear in practice if there is a considerable separation of time scales between the processes intended to be included in the internal variability of climate and those intended to be (at least partially) excluded from it, and if initialization is chosen sufficiently far (relative to the fast former processes) but not too far (relative to the slow latter processes) in the past. However, we will then recover the conditional definition corresponding to the natural probability measure of the fast subsystem, and initialization by observations (assuming it is possible) will be relevant only in the slow variables. The conditional definition motivated by the concept of snapshot attractors and that of DelSole and Tippett (2018) based on observations become special cases of each other in this situation. Note, however, the ambiguity that may arise about how to initialize the slow variables if no reliable instrumental records are available.

A further problem is posed by regime behavior (e.g., Franzke et al. 2015) in the slow variables even if the separation of time scales is sufficiently large from a practical point of view for most initializations. In particular, if initialization takes place during a regime transition, the evolving
probability density may become strongly dependent on its initial condition even on a short time
scale in the sense of how it is distributed between the two regimes in the slow variables (how many
ensemble members fall into one regime or the other in a numerical investigation); and, according
to the slow subsequent evolution, uniqueness may only be reached on the time scale of the slow
variables. That is, uniqueness and thus a sound definition of climate will be lost on a short time
scale. See Appendix 5 for a numerical illustration in a two-variable toy model where internal
variability is modeled by stochastic terms.

An even further issue can be the presence of multiple stationary chaotic attractors with intertwined
basins of attraction, possibly including riddled basins (Alexander et al. 1992), and rate-dependent
tipping (Ashwin et al. 2012) between them. In such a case, different initial densities will not
converge even if their difference is small, i.e., uniqueness will again be lost.

One should also note that a chaotic snapshot attractor can split in the case of an underlying rate-
dependent tipping (Kaszás et al. 2019), and only one of the branches will be relevant if observations
for initialization are available after the splitting. Although the individual branches do not have
their own, separate basins of attraction in the infinitely remote past, one can select those ensemble
members that end up on the relevant branch, as in Kaszás et al. (2019).

The discussion has so far concerned mainly how the presence of processes with different time
scales affects a possible practical definition of climate, based on how much corresponding vari-
ability unfolds on a time scale of practical interest. However, even if this unfolding proves to be
negligible for certain processes, the variables associated with these processes are supposed (and
must be ensured in numerics) to sample the attractor: in the opposite case, the probability density
traced out by the ensemble in the rest of the variables may also be affected in an undesirable way.
This situation may arise, e.g., in an incomplete spin-up from off-attractor initial conditions. (More
generally, model drift (Gupta et al. 2013) should be avoided between the initialization of different
ensemble members, or should be corrected for in some way.)

For cases when slow processes do play a role by influencing the time evolution of the practically
relevant probability density (traced out by an ensemble), i.e., one already converged in the faster
variables, we must emphasize that this is, if uniqueness is preserved, a climate change (according
to the conditional definition of climate) but is not (entirely) a forced response (as it does not
originate (only) from an explicit time dependence of the equations of motion): the two concepts
decouple in such situations. A forced response can only be identified relative to the time evolution observed in the absence of any time dependence in the relevant terms of the equations of motion. It is, however, left as a question for future investigation if uniqueness can be preserved in cases as described: perhaps the time evolution of slower processes will exhibit unpredictability from the very first moment of initialization, possibly as a result of interaction with faster processes. See some hints on this issue in Hawkins et al. (2016). In relation to Hawkins et al. (2016), especially points 2 and 4 in their summary section, it should also be mentioned that the implicit notion of an unforced climate change induced by variations in slower system components already exists; cf. the discussion about possible gaps in the spectrum of the relevant operator in the next section.

4. Time scales and system components; further practical issues

Since a major separation of time scales is not obvious in the real Earth system and in realistic models thereof, at present we are not able to assess how precisely the (possibly conditional) definition based on the natural probability measure of a snapshot attractor is applicable to these systems. The concept nevertheless gives guidance to decide what can be regarded climate and what cannot in a given study or some wider field of research.

This is illustrated by the example of the ocean, which is one influential source of long time scales in the Earth system. Studies suggest that time scales associated with the mixed layer and with layers below the thermocline are separated by a factor of about 10, and there might be no other characteristic time scale in between (e.g., Li and Jarvis 2009; Olivié et al. 2012). (Note that an apparent continuous dependence of the time scale on depth (Yang and Zhu 2011) may well be a spurious result of an interplay between the two mentioned time scales.) This separation might or might not be just enough to treat the deep ocean separately from the rest of the system: by the time “complete” variability would be unfolded in the mixed layer, variations in the deep ocean might just become large enough to be relevant for an appropriate description.

Note that reaching “complete” variability must always be defined in terms of some practical criterion, according to the exponential-like nature of convergence. The distance from a suitably defined probability measure may generally be thought to become negligible after a few times the longest relevant time scale passes from initialization.
In the particular case of the ocean, as mentioned, one characteristic time scale of the unfolding of variability is a few decades (e.g., Li and Jarvis 2009; Olivié et al. 2012), so that even conditional definitions of climate must rely on this unfolding in century-long studies of the Earth system. In terms of the definition of DelSole and Tippett (2018), a lead time of a few decades is required at least, and any shorter choice will inhibit an appropriate interpretation of corresponding results. Note, however, that whether the unfolding of variability on longer time scales is required to be taken into account remains an open question. Even though the separation by a factor of 10 gives some hope that the answer is ‘no’, it is unclear why the intermediate time scale of the Atlantic Multidecadal Oscillation/Atlantic Multidecadal Variability (e.g., Delworth et al. 2007), if such a mode exists (Vincze and Jánosi 2011; Mann et al. 2021), does not appear in the referenced analyses and what role it plays in the unfolding of variability. We emphasize it here that the numerically observable time scales may depend on the choice of the variable.

Obviously, processes of the Earth system without influence from or influence on global atmospheric and oceanic circulation and thermodynamics (e.g., tectonics and perhaps small-scale hydrodynamics, respectively) should not be considered part of climate. One may also think of situations with little correlation between fluctuations of different system components, for which an example might be the relationship between the deep ocean and the surface-related processes, in which case the unfolding of deep oceanic variability would be irrelevant for most observables of practical interest. According to most recent research (Singh et al. 2022), there are some signs that this is so for most of the globe but not for the Southern Ocean.

From the point of view of convergence of probability densities, identifying the slow components and the corresponding time scales (as far as a given time scale is associated with a given system component), and the degree of correlation between their internal variability should in principle rely on the spectral theory of transfer operators (Lasota and Mackey 1994; Slegers 2019): in the absence of explicit time dependence and under appropriate conditions, time scales of convergence correspond to eigenvalues of the transfer operator of the system, while slow components are related to its eigenfunctions (Györgyi and Szépfalusy 1988; Navarra et al. 2021); and generalization to time-dependent systems is possible (Froyland et al. 2010). See Appendix 5 for more details.

One also has to consider the possibility that the real Earth system or some realistic model thereof does not meet the prerequisites of the description of convergence mentioned above. Long-term
persistence (polynomially decaying autocorrelation) and, more generally, scaling of fluctuations in climate-related time series are reviewed by Franzke et al. (2020). As pointed out in their sections 2.3 and 5, long-term persistence and scaling may be illusory or they may result from external forcing, which would be in harmony with the Markovian nature of (most) equations of motion. (Note that the Hurst effect does not imply long-term persistence (Franzke et al. 2015).) In any case, if there is a break in the power spectrum such that there is a non-scaling regime of considerable length beyond the break (as, e.g., in Vincze and Jánosi 2011), the decomposition of the convergence to eigenmodes (as described in Appendix 5) may retain its pertinence.

As discussed in Section 3, regime behavior and intertwined basins of attraction can also inhibit defining climate due to a lack of uniqueness. However, the absence of different qualitative behaviors in global variables between members of currently existing large ensembles suggests that such effects are restricted to particular system components at most. Such effects might nevertheless appear in some slow system components (possible examples are related to Labrador Sea ice cover (Danabasoglu et al. 2020) and Southern Ocean variability (Gnanadesikan et al. 2020)), and uniqueness might or might not be lost in these cases: it depends on the way or the time of initialization. Cf. the illustration in Appendix 5 for the case of regime transitions; as for intertwined basins of attraction, they are unlikely to play a role if initialization is performed by means of a small perturbation of a configuration on an attractor.

Taken together, we can say that distinguishing between different time scales of convergence appears to presumably provide a sound definition of climate in the sense of Section 3: from the point of view of century-long investigations and as discussed at the beginning of the current Section, we might hope to be able to meaningfully define climate through the probability measure obtained after a convergence time of a few decades. Further gaps in the spectrum of time scales may possibly give rise to sound definitions for investigations on other time scales, but whether such gaps exist is an open question at present. Note that paleoclimatic studies may well rely on different time scales and thus on a different definition of climate compared to century-scale projections.

While the potential relevance of separation between time scales in formulating a practically satisfying definition of climate was already discussed by Lorenz (1975) and was maybe born together with the first attempts to define climate, note that times scales of convergence are concerned in the conditional definition formulated in the Section 3. As a consequence, this definition allows
external forcing to induce climate changes on arbitrarily short time scales (e.g., after volcanic eruptions), irrespective of possible slower components of internal variability.

5. Conclusions; a proposal for an initialization scheme

As a summary, an operational definition of climate, in the context of century-long studies at least, should presumably rely on a decadal-scale convergence of an ensemble (which is infinitely large in principle but is sampled by a finite number of members in numerical modeling) within a basin of attraction to an (approximately) unique but time-dependent probability density: this density would be identified with climate. In case slower system components can play a considerable role in determining this (approximately) unique probability density, which thus becomes conditional on the state of the given slower system components, this definition assumes

(a) a sufficiently large separation between the relevant time scales, and

(b) the avoidance of a regime transition in the given slower system components at initialization.

For such a case, we spell out two issues that require further attention.

(i) The initialization of the given slower system components should rely on their observed configuration. Note that this is not so in current practice, but initial conditions in slower system components rely on one or more arbitrary time instants of a long spin-up run: this may be problematic from a practical point of view regardless of how climate is defined.

(ii) The concept of climate change may decouple from that of the forced response.

In a given model subjected to a given forcing (i.e., a given form of time dependence), it is actually possible to decide if an (approximately) unique probability density generally appears on the time scale of the faster variables and to assess the role of slower system components in an affirmative case. We propose the following ensemble initialization scheme, pictured in Fig. 3, for this purpose.

In the first step, two ensembles, Ef1+ and Ef1−, are micro-initialized (Hawkins et al. 2016) around a chosen point in a long control run. The difference between their initialization times should be small enough to ensure the fastest slow variables (with time scales on the order of a century in century-scale studies) to be approximately the same at the beginning. Meanwhile, these two ensembles should realize fairly different initial states in the slowest fast variables (with
Fig. 3. Illustration of the initialization scheme proposed in the main text. 10-year running mean of the global mean surface temperature is plotted as a function of time; data are from V. Lembo (2020, unpublished data) and are described in Lembo et al. (2020). Vertical lines denote years for the initialization of individual ensembles, and markers denote corresponding values of the temperature (coinciding for forced and unforced ensembles). Note that initialization should be based on some given model state within the marked years.

Time scales on the order of a decade in century-scale studies). One could either guess what such a variable is, or artificially create a low-passed time series of a certainly faster variable (as in Fig. 3) in the hope that fluctuations in such time series correspond to differences in the slowest fast variables. To ensure sufficient difference and decorrelation in the slowest fast variables, $\text{Ef1}^+$ should be initialized at a time of a local maximum of the chosen fast variable, and $\text{Ef1}^-$ at a local minimum as far in time as possible such that the difference in time can still be regarded much smaller than the time scale of the fastest slow variables. The trajectories are then integrated under the same forcing of interest, typically the historical forcing followed by some future scenario like SSP3-7.0 (Gidden et al. 2019). In the second step, this procedure is repeated for a few further pairs of ensembles, $\text{Ef2}^+/−, \text{Ef3}^+/−$, etc.

The absence of a practically complete convergence of $\text{Ef}x^+$ and $\text{Ef}x^−$ to each other on the time scale of the slowest fast variables implies (a) the inapplicability of the conditional definition of climate if all x’s are concerned [possibly because of processes with an intermediate time scale like perhaps the Atlantic Meridional Overturning Circulation (AMOC); cf. Buckley and Marshall (2016); Hawkins et al. (2016); Blaschke et al. (2022)], and (b) the problem of regime transitions if only some. If the convergence is practically complete on the mentioned time scale for most
x’s, a comparison between different x’s shows if the (approximately) unique probability density is conditional on the slow variables. Remember that issue (i) is implied if this is so.

Issue (ii), on the other hand, can be investigated in a third step, by comparing the ensemble simulations introduced so far, $E_{fx} \pm$, to those generated with identical initialization but with no forcing ($E_{ux} \pm$; ‘f’ and ‘u’ stand for forced and unforced, respectively). Note, however, that model drift (Gupta et al. 2013) has the same effect from this point of view as slower system components, but, at least, forced changes can always be discerned. Comparing $E_{ux+}$ and $E_{ux-}$ provides information about the effect of forcing on convergence.

If providing a sound definition of climate is impeded by problem (a), there is still a possibility to treat climate predictions similarly to probabilistic (ensemble) weather forecasts (Gneiting and Raftery 2005), i.e., to associate probabilities to different outcomes based on the present state of faster variables and the uncertainty in this knowledge (leading to what is discussed by DelSole and Tippett 2018). The actual conclusions drawn from the above-sketched investigation may also depend on the particular choice of observable to study.

Our proposed initialization scheme is different from that of Hawkins et al. (2016), the CanESM2 large ensemble (Kirchmeier-Young et al. 2017; Singh et al. 2022) and the CESM2 large ensemble (Rodgers et al. 2021) in that pairs of micro-initialized ensembles are initialized for each state of any system component slower than the time scale of the slowest fast variables (e.g., slower than the upper ocean, having a decadal time scale, in century-scale studies; note that the strength of AMOC might be too slow to be regarded as the slowest fast variable). This is the key for enabling the assessment of convergence to a (possibly conditionally) unique probability distribution. Furthermore, the different pairs should ideally be initialized sufficiently far away from each other to ensure decorrelation in deep oceanic internal variability, i.e., farther away than just 50 years (as in the cited studies). Model drift (as in Singh et al. 2022) is not at all ideal for assessing the impact of slower system components due to its inherently artificial nature. If differences in slower system components are supplied by their internal variability, a statistically sound evaluation of a full ensemble of micro-initialized ensemble pairs becomes possible. The particular statistical techniques are yet to be explored (for some first attempts, see Singh et al. 2022).

It should be emphasized that it is always “safe”, from the point of view of practical relevance, to initialize the slower system components according to observations (but note the problem of the
initialization shock (e.g., Doblas-Reyes et al. 2011)), in which case a single +/− ensemble pair is sufficient for the investigation of convergence. However, if appropriate observations are not available (as is presumably the case for the deep ocean), generating ensembles with different x’s are important for the purpose of mapping out different possibilities permitted by the system.

The picture is presumably much simpler for studies concerning time scales much longer than a century (e.g., those about paleoclimate), in which convergence in all system components may be necessary to ensure.

One undesirable property of any ensemble-based definition of climate is its inaccessibility in single realizations (including the observed evolution of the real Earth system), but note that such an accessibility is not actually required in a probabilistic framework [unlike Werndl (2016) suggests].

We emphasize that according to such a definition, as long as the underlying probability density remains (approximately) unique, internal variability will not be a source of uncertainty in the description of climate, not even when its future projections are considered. Instead, the very definition of climate should correspond to a full description of the (possibly conditional) statistics of the system in terms of the mentioned probability density, including the statistics of internal variability.

In practice, this means that all statistical quantifiers should be evaluated with respect to the ensemble. This also implies that there is no need to “invent” newer and newer ensemble-based statistical quantifiers [like correlation coefficients (Herein et al. 2017), empirical orthogonal functions (Haszpra et al. 2020), etc.] individually, one by one: instead, one should just follow this “recipe” for the evaluation of any statistics. This does not exclude evaluating ensemble-wise statistics of statistical quantifiers evaluated over time intervals in single realizations (“interval-wise taken” ensemble statistics in Drótos et al. 2015) — however, evaluating a statistical quantifier over a time interval and taking its ensemble mean is not the correct way to learn about the given statistical quantifier from a probabilistic point of view. This is related to the violation of Birkhoff’s ergodic theorem in a system with explicit dependence on time (Drótos et al. 2016); as a practical example, sources of nonergodicity for teleconnections as cross-correlations are analyzed in Bódai et al. (2022).
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**Data availability statement.** The data presented in Figs. 1 and 2 are from Drotos (2022). The data used for the creation of Fig. 3 were shared by V. Lembo (2020, unpublished data) and are described in Lembo et al. (2020). The data presented in Fig. B1 were created by Bodai (2022).

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**APPENDIX A**

**Identifying time scales of convergence**

We discuss here how the spectral theory of transfer operators (Lasota and Mackey 1994; Slegers 2019) enables one to identify slow system components and corresponding time scales of convergence.

Let us first consider an autonomous system, i.e., one without any explicit dependence on time, hypothetically describing a stationary climate:

\[
\dot{x} = F(x), \tag{A1}
\]

where \(x \in X\) represents the vector composed of all dynamical variables of the system, with \(X\) being the \(d\)-dimensional phase space spanned by these vectors, and \(F\) defines the dynamics, which
is assumed to be dissipative. Let $\mathcal{P}_{t_0}^t$ denote the Ruelle–Perron–Frobenius or transfer operator associated with the dynamics between time $t_0$ and $t_0 + t$ with $t \geq 0$ and defined with respect to the Lebesgue measure of $X$: the time evolution of probability densities $f$ defined on $X$ is described by the action of operators $\mathcal{P}_{t_0}^t$ on $f$ with different values of $t \geq 0$. If the operators $\mathcal{P}_{t_0}^t$ are quasi-compact (i.e., if they have a finite number of isolated eigenvalues outside the essential radius, which we hope to be the typical case), the time evolution of an arbitrarily initialized probability density $f$ from the class of square-integrable functions on $X$ can be decomposed as

$$\mathcal{P}_{t_0}^t (f) = \sum_{i=1}^{N} c_i \lambda_i^{t/T} \varphi_i + r(t), \quad (A2)$$

where

$$c_i = \frac{\int_X \frac{f(x) \varphi_i(x)}{\varphi_1(x)} d^d x}{\int_X \frac{\varphi_i(x)^2}{\varphi_1(x)^2} d^d x} \quad (A3)$$

(note that $c_1 = 1$), $T$ is the unit of time, $N$ is the number of isolated eigenvalues of the operator $\mathcal{P}_{t_0}^T$, $\lambda_i$ is the $i$th eigenvalue of the operator $\mathcal{P}_{t_0}^T$ with $|\lambda_1| = 1$ and $|\lambda_i| < 1$ for all $1 < i \leq N$, $\varphi_i$ is the $i$th eigenfunction of the same operator (note that $\varphi_1$ is the density of the natural probability measure), $r(t)$ is a residual decaying faster than $\lambda_1^{t/T}$ (Györgyi and Szépfalusy 1988; Slegers 2019; Navarra et al. 2021). If there are multiple attractors, which have separate basins of attraction in the phase space, the decomposition (A2) applies separately to densities $f$ with an initial support falling in a single basin (Tantet et al. 2018a).

Eq. (A2) means that $f$ converges to the density $\varphi_1$ of the corresponding natural probability measure, and the convergence proceeds according to exponential terms with different time scales and a fast-decaying residual. The exponential contributions with different time scales may then form the basis of the conditional definition of climate: if the separation between time scales is sufficiently large, “complete” convergence is possible on one time scale without an influence from processes with longer time scales.

Note that a time scale of convergence may be regarded to be associated with a particular system component if the corresponding eigenfunction depends strongly on the variables associated with the given system component but depends much less on other variables. Furthermore, the multivariate distribution shows how much fluctuations in different system components are correlated.
While the above considerations concern autonomous systems, generalization to periodically forced systems is easy by identifying the unit $T$ of time with the period of the forcing. In this case, Eq. (A2) will hold for $t = nT$ with $n \in \mathbb{N}$. Similar results also exist in systems with nonperiodic dependence on time (Froyland et al. 2010), but the eigenvalues are not constant in this case. Although tipplings (Ashwin et al. 2012), especially crises of corresponding stationary chaotic attractors (Tantet et al. 2018b), may lead to complications at least for eigenvalues associated with some particular system component, if most of the eigenvalues vary moderately enough, as might be expected under forcing scenarios relevant for century-long investigations, these eigenvalues remain informative about the time scales in the system. An attempt for computing an approximation of the spectrum of the relevant transfer operator (or the application of more sophisticated techniques (Froyland et al. 2014, 2016)) is nevertheless beyond the scope of this article.

**APPENDIX B**

**Regime transitions and uniqueness in slow-fast systems**

We use the stochastic (in the Itô sense) slow-fast system

\[
\begin{align*}
dx &= (-x^3 + 2x)dt + \sigma_{xx}dW_{xx,t} + \frac{1}{\epsilon}\sigma_{xy}yd\tau, \\
dy &= \frac{1}{\epsilon x^2}(-y + cx)dt + \frac{1}{\epsilon}\sigma_{yy}dW_{yy,t},
\end{align*}
\]

(B1)

(B2)

to demonstrate that an ensemble micro-initialized during a regime transition cannot represent climate in the absence of its uniqueness on the short term. A time scale separation between the slow $x$ and fast $y$ variables is achieved as $\epsilon \to 0$ (Wouters and Gottwald 2019). To represent a practical, realistic situation, we set $\epsilon = 0.2$. The slow system is characterized by a symmetric quartic polynomial like in Bódai (2020). It is perturbed both by some noise ($\sigma_{xx} > 0$) and the fast system ($\sigma_{xy} > 0$), which latter features (internal) variability generated by white noise ($\sigma_{yy} > 0$) (Hasselmann 1976; Wouters and Gottwald 2019). Effectively, the time scale separation between $y$ and some even faster $z$ whose governing equation is eliminated is readily represented in the stochastic model. The noise $dW_{xx,t}$ is the slow system’s own internal variability unaffected by the fast system. The fast variable is affected by the slow variable ($c \neq 0$), which is why when the climate cannot be defined wrt. the slow variable, it carries over to the fast one. We use the
parameter values of: $\sigma_{xx} = 0.6$, $\sigma_{xy} = 0.4$, $\sigma_{yy} = 1$, $c = 0.2$. The equations are integrated by the Euler–Maruyama integration scheme, using a time step of $\Delta t = 0.02$.

The quartic polynomial represents a double-well potential function and so gives rise to a saddle-type unstable fixed point, a saddle, at $x = y = 0$ in the unperturbed ($\sigma_{xx} = \sigma_{yy} = 0$) 2D system (B1)-(B2), also called a Melancholia state in Lucarini and Bódai (2020), whose stable manifold makes a finite angle with the $x = 0$ line owing to the coupling $\sigma_{xy} > 0$. With a weak perturbation (in the sense of Bódai (2020)), infrequent transitions between the potential wells, across the Melancholia state, take place in terms of a long single-realization “control” run. In order to examine the uniqueness of the converged ensemble, we micro-initialize a pair of ensembles at some state of the control run. Namely, we “perturb” the fast variable as $y + \delta y$, $\delta y = +1$ for one ensemble and $\delta y = -1$ for the other ensemble. (Such a “perturbation” of a state for the purpose of generating initial conditions for trajectories is not to be confused with the “dynamic perturbation” of trajectories under the evolution equations as a result of $\sigma_{xy} > 0$, etc., in (B1)-(B2).) If “micro-initialization” meant to simply contrast the concept of “macro-initialization”, then it should mean a concentration of initial conditions simply with respect to the slow variable $x$. However, it seems that its common implementation constitutes a concentration also wrt. the fast variables, $y$ and also even $z$ (Deser et al. 2020), which is certainly a natural and cautious choice. We utilise the concentration wrt. $y$ in order to have two markedly different ensembles initially. When the dynamics is deterministic, a minute mismatch of the initial conditions within one of the ensembles — at least wrt. $z$ — is needed for the spread of that ensemble. In our stochastic modeling, however, it is clearly not required. The various different realizations of the ensemble members are generated by various different realizations of the Wiener process $W_{yy,t}$. Note that the standard deviation $\text{std}[y]$ is comparable with $|\delta y| = 1$, and so the applied perturbations can correspond to extreme opposite, or, rather different, states of the fast process. Given the said inclination of the stable manifold, which is the basin boundary of the unperturbed system, the opposite perturbations $y \pm \delta y$, even if taken in the $y$-direction only, could already achieve the placement of the two initial conditions in the different basins of attraction, provided that the current $(x, y)$ was not far off from the basin boundary. Then, ensuing perturbed ($\sigma_{yy} > 0$) realizations will much more likely end up in the near future in the potential well/regime where they started out from. As only the fast variable is perturbed to micro-initialize an ensemble, the same single realization of $W_{xx,t}$ of the control run
is used for all the ensemble members. In effect, this gives rise to nonautonomous dynamics, i.e., explicit time dependence in the system. Therefore, it is the stable manifold of the corresponding snapshot saddle that will actually control the transitions (Bódai et al. 2013).

When we initialize two ensembles during a transition (see the middle row of Fig. B1), the ensemble means of either the fast or the slow variable, $\langle y \rangle$ or $\langle x \rangle$, do not converge but remain well separated, indicating the lack of uniqueness, at least on the time scale of the fast variable $y$. I.e., the realized ensemble will depend on the particular initialization of the fast system. This indeed prevents any of these to objectively represent climate. To the contrary, when we initialize two ensembles sufficiently far away from a transition, whether right before or after it (see the top and bottom rows of Fig. B1, respectively), the ensemble means converge on the time scale of the fast variable, indicating uniqueness. Due to the “forcing” by the slow system, $W_{xx,t}$, clusters of trajectories (a subset of all trajectories because of $\sigma_{xy} > 0$) suffer a regime transition in a coordinated manner, which is imprinted on the evolution of the ensemble means. That is, had the toy model reflected realistic characteristics of the climate system, regime transitions of the slow system could give rise to the delineation of the concepts of climate change and forced response.

The case of $\sigma_{xx} = 0$, when the slow system does not have an internal variability in isolation from the $y$ system component, is qualitatively similar: there is no uniqueness on the fast time scale in association with initialization during a regime transition of $x$.

References


Fig. B1. Initialization during or away from a regime transition precludes or supports the definition of climate, respectively. Two ensembles are micro-initialized by perturbing the fast variable as $y + \delta y, \delta y = +1$ or $-1$ (see main text), upon which the ensemble means $\langle y \rangle$ or $\langle x \rangle$ are plotted in diagrams on the left to examine convergence, using 1000 ensemble members each ensemble. Diagrams in the middle column provide zoomed pictures of those on the left wrt. time, excluding the $y$ control time series, for the better visibility of uniqueness. The legend annotations in two panels apply to all in the left and middle columns. On the right, spaghetti diagrams of all the 1000 slow time series are given for one of the ensembles ($\delta y = +1$). Data were produced by code by Bodai (2022).


