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Insights from Earth system model initial-condition large ensembles and future prospects

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Internal variability in the climate system confounds assessment of human-induced climate change and imposes irreducible limits on the accuracy of climate change projections, especially at regional and decadal scales. A new collection of initial-condition large ensembles (LEs) generated with seven Earth system models under historical and future radiative forcing scenarios provides new insights into uncertainties due to internal variability versus model differences. These data enhance the assessment of climate change risks, including extreme events, and offer a powerful testbed for new methodologies aimed at separating forced signals from internal variability in the observational record. Opportunities and challenges confronting the design and dissemination of future LEs, including increased spatial resolution and model complexity alongside emerging Earth system applications, are discussed.

Identifying anthropogenic influences on weather and climate amidst the background of internal variability, and providing robust projections, are central scientific challenges with practical implications[1–6]. Since the inception of the Coupled Model Intercomparison Project (CMIP), substantial progress has been made on quantifying sources of uncertainty in climate projections (for examples, see refs. [7–9]). However, such multi-model archives confound uncertainties arising from differences in model formulation (that is, structural uncertainty) with those generated by internal variability (variability from natural processes in the coupled ocean–atmosphere–land–biosphere–cryosphere system). This distinction is important because the former is potentially reducible as models improve, whereas the latter is an intrinsic property of each model and is largely irreducible after the memory of initial conditions is lost, typically after less than a few years over land[10]. This key distinction is often not widely appreciated and communicated to stakeholder groups[11]. Indeed, internal variability accounts for approximately half of the inter-model spread within CMIP for projected changes in near-surface air temperature, precipitation and runoff across North America and Europe over the next 50 years[5,8,9,12–14].

One way to isolate the uncertainty from internal variability is to create an ensemble of simulations with a single climate model under a particular radiative forcing scenario, applying perturbations to the initial conditions of each member to create diverging weather and climate trajectories, causing ensemble spread (for examples, see refs. [12,15–17]). Since the resulting sequences of unpredictable internal variability are randomly phased between the individual ensemble members, the forced response can be estimated by averaging over a sufficient number of members. The definition of 'sufficient' depends on the quantity of interest, location, spatial scale, temporal scale and time horizon, often on the order of 10–100 members (for example, see ref. [12]). Such 'initial-condition large ensembles (LEs)' conducted with fully-coupled global models are a relatively new development in climate science, with the first efforts employing CMIP3-era models[12,18].

The past few years have witnessed an explosion of LEs with newer-generation CMIP5-class Earth system models (ESMs; Table 1). Each LE required substantial high-performance computing resources and generated hundreds of terabytes of output. For example, the CESM1-LE used 21 million CPU hours and produced over 600 terabytes of model output (for comparison, the entire CESM1 contribution to CMIP5 was 170 terabytes). Making these 'big data' projects accessible to a wide range of users is challenging, yet their ease-of-use for different types of analysis workflows has a substantial impact on the scientific value gained from their production. A case in point is the NCAR CESM1-LE Project[19], which was created to serve a broad research community by responding to user needs to provide easy access to the output and stable on-disk access. This project has resulted in more than 860 peer-reviewed studies to date, with approximately 400,000 data files downloaded. Remaining nimble to new workflows and users is important, as is following the

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Table 1 | The multi-model LE archive and data repository

Modelling centre	Model version	Resolution (atmosphere/ocean)	Years	Initialization	No. of members	Forcing	Reference
CCCma	CanESM2	~2.8°×2.8°/~1.4°×0.9°	1950-2100	Macro and micro	50	Historical, RCP 8.5	94
CSIRO	MK3.6	~1.9°×1.9°/~1.9°×1.0°	1850–2100	Macro	30	Historical, RCP 8.5	95
GFDL	ESM2M	2.0°×2.5°/1.0°×0.9°	1950–2100	Macro	30	Historical, RCP 8.5	78
GFDL	CM3	2.0°×2.5°/1.0°×0.9°	1920–2100	Micro	20	Historical, RCP 8.5	96
MPI	MPI-ESM-LR	~1.9°×1.9°/nominal 1.5°	1850–2100	Macro	100	Historical, RCP 2.6, RCP 4.5, RCP 8.5	61
NCAR	CESM1	~1.3°×0.9°/nominal 1.0°	1920–2100	Micro	40	Historical, RCP 8.5	97
SMHI or KNMI	EC-Earth	~1.1°×1.1°/nominal 1.0°	1860–2100	Micro	16	Historical, RCP 8.5	98

Salient characteristics of each LE, including the method of initialization. Here, the term 'micro', referring to micro perturbation[15], indicates that all LE members begin from a single coupled model state, with slight perturbations introduced only in the atmospheric component to create ensemble spread. The term 'macro', referring to macro perturbation[15], indicates that the LE members begin from a variety of coupled model states (for example, from different years in a long control simulation). Canadian Earth System Model (CanESM2) consists of a hybrid approach, with ten micro ensemble members for each five macro ensemble members. Additionally, 'forcing' refers to the greenhouse gas concentrations used to drive the model simulations; 'historical' corresponds to observed forcing during the historical period; and representative concentration pathway (RCP) refers to the estimated trajectory of greenhouse gas emissions corresponding to a range of radiative forcing values of 2.6 W m^{-2}, 4.5 W m^{-2} and 8.5 W m^{-2} by 2100. Data from the multi-model LE archive are accessbible from ref. [22].

recommended big data practice of 'bringing your analysis to your data'. Following these principles, the CESM1-LE was made freely available as a public dataset on the Amazon Web Services cloud in October 2019. Access on the commercial cloud demonstrates strong interest in LEs from industry and scientific communities well beyond typical climate researchers. Such scrutiny and widespread use attests to the value of LEs for a range of applications—truly a sea change for climate and related sciences.

Strength in numbers with a Multi-Model Large Ensemble Archive

While a single-model LE has enormous utility, a multi-model collection of LEs can be leveraged for robust comparison of both the forced response on regional or decadal scales across models and internal variability across models. It can also advance model evaluation by providing more complete information on biases in internal variability versus those in the forced response. Unlike CMIP, a multi-model archive of LEs allows for direct separation of projection uncertainty into a structural component due to model differences and an internal variability component. Despite these advantages, most analyses to date have been limited to one or two LEs (with a few exceptions; for examples, see refs. [20,21]), in part because of the burdensome task of accessing large volumes of data from disparate sources. To fill this gap, we have produced a centralized data repository of LEs conducted with seven different CMIP5-class ESMs under historical and future emissions scenarios (hereafter referred to as the 'Multi-Model Large Ensemble Archive' (MMLEA); Table 1). This repository includes gridded fields of key variables at daily and monthly resolution, and it is easily accessible via the National Center for Atmospheric Research (NCAR) Climate Data Gateway[22].

This Perspective seeks to illustrate what MMLEA can offer, with the aim of widening its usage and stimulating new research directions and Earth system applications. We also look to the future of initial-condition LEs, in particular the opportunities and challenges that confront their design and facilitate their accessibility to the user community. In this regard, we offer a path forward that balances demands for increased spatial resolution and model complexity against ensemble size. We encourage future CMIPs to take on a greater role in the design and coordination of LE simulations, data storage and access.

New insights on separating sources of uncertainties

Individual LEs have been crucial to understand the need to consider internal variability alongside forced trends in past and future climate change at continental and smaller spatial scales[10,12,14,19,23–31]. The MMLEA expands on this view by providing new insights on the relative roles of internal variability and model structural differences—two sources of projection uncertainty in addition to the radiative forcing scenario. The MMLEA shows both factors can play a first-order role in the magnitude and pattern of warming at continental scales; for example, the distributions of trends in North American air temperature over the last 60 years from each of the seven LEs (Fig. 1 and Methods). While they all encompass the observed trend value, they clearly differ in the strength of the forced trend (given by the ensemble mean) and in the shape and width of the distribution of trends, which emerge due to internal variability. This information on model dependence of both the forced trend and its range due to internal variability is unique to the MMLEA and could not have been deduced directly from CMIP archives. It is important to note that a LE centred on the single observed trend value does not constitute evidence that this particular model is more realistic than any other model (see further discussion in sub-section titled 'Multi-model LEs as methodological testbeds for observations' below).

The distribution of North American temperature trends based on CMIP5 (see Methods) is only slightly wider than that based on an individual LE and is due to both model differences and internal variability (see grey shaded probability distribution function (PDF) (Fig. 1)). Moreover, the MMLEA spans a wider range than CMIP5, suggesting that CMIP5 under-samples internal variability at regional scales. This highlights the importance of evaluating the realism of models' internal variability of trends, since a model with unrealistically large trend variability (that is, a broad distribution) can encompass the observed trend for the wrong reason and would also inflate uncertainty in projections. Approaches to address this challenge are discussed in the sub-section titled 'Multi-model LEs as methodological testbeds for observations' below.

Just as North American temperature trends vary across the members of a LE, the geographical pattern of trends can also differ strikingly (Fig. 1). This can confound comparisons of individual simulations from different models and lead to erroneous interpretations, since internal variability might be mistaken for structural differences. With enough members, the spatial pattern of the forced response emerges for each model, allowing for a direct comparison between models. Models may show similar forced patterns of poleward-amplified warming but different overall amplitudes (Fig. 1), a conclusion that is difficult to discern without a MMLEA. Similar issues confront the study of observed real-world trends (Fig. 1), since these are also just one realization of many that could have happened (see sub-section titled 'Multi-model LEs as methodological testbeds for observations' below).

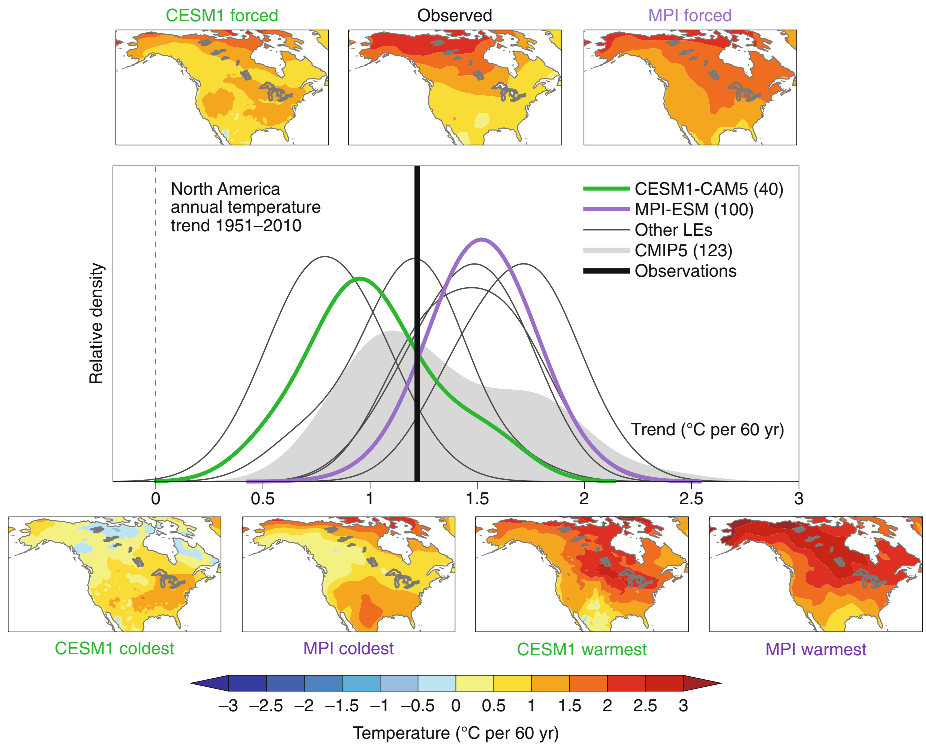

Fig. 1 | Internal variability and model differences in continental temperature trends. The distribution of 60-yr annual temperature trends (1951–2010) over North America (24–72° N, 180–62° W) from seven ESM LEs (thin curves), 40 different CMIP5 models (grey shading), and observations (Berkeley Earth Surface Temperature; vertical black line). The maps show the associated patterns of temperature trends: top row, observed and the forced component (estimated by the ensemble mean) from two LEs (CESM1 in green and MPI in purple); bottom row, individual ensemble members from CESM1 (green) and MPI (purple) with the weakest ('coldest') and strongest ('warmest') trends. Note that the individual member maps show the total (forced-plus-internal) trends in the model LEs. Observed trends are analogous to an individual ensemble member in that they reflect forced and internal contributions.

Quantifying model uncertainty requires knowledge of the forced response in each model, but most models in past and current CMIPs do not have enough available ensemble members to allow for a robust estimate of the forced response. Instead, low-frequency statistical fits to a single ensemble member are often used to estimate the forced response (for examples, see refs. [8,9]). Consequently, internal variability has to be estimated either from the residual of this fit or from long pre-industrial control simulations. From these approaches, it is often not easy or possible to robustly estimate systematic changes to internal variability under increasing radiative forcing. The availability of a MMLEA circumvents these limitations and assumptions. More importantly, it allows one to separate the sources of uncertainty at smaller spatial and temporal scales, and for quantities that are notoriously variable, such as precipitation and extremes.

Decision-making and risk assessment in a variable climate

LEs are increasingly proving their utility in the context of real-world decision-making[32] where full assessment of changing climate risks is needed, including variability and extremes. In particular, discerning changes in variability and extremes requires large sample sizes[33–37]: the hallmark of LEs. Moreover, the MMLEA is critical for evaluating the extent to which projected changes in variability and extremes are model-dependent.

The Upper Colorado River basin—which feeds the largest reservoirs in the US—is an example of where changes in mean and variability can produce a wide range of climate risks for water managers. This basin is located at a latitude where projected changes in precipitation are notoriously uncertain: the transition zone between the expected drying in the subtropics and the wetting at high latitudes[2,38–40]. The MMLEA shows divergent outcomes regarding how decadal mean precipitation will change in this region under a high-emissions scenario (Fig. 2a). However, decadal variability of precipitation is projected to increase on average by ~10% of the magnitude of the forced change (Fig. 2b). This result by itself suggests a heightened hazard of prolonged droughts and pluvials and could, in the absence of consistent projections of mean change, provide useful information for refining water management strategies.

To illustrate the challenge of projecting extreme events, we use an example of daily summer heat extremes for a location in the south-central US centred on Dallas, Texas (see Methods). As expected under global warming, daily July heat extremes at Dallas are projected to increase over the twenty-first century; however, their evolution is far from monotonic in any single ensemble member, and their rate and degree of increase varies considerably across different realizations of future internal variability in the same model (Fig. 3a). For instance, historical daily heat records could be broken almost continuously starting in the late 2060s, or their occurrence could be more punctuated, with some decades even as late as the 2090s spared from any days of record heat depending on how internal variability unfolds (Fig. 3a). This variety of temporal expressions of historical heat extreme exceedances should be a cautionary note on the enormous impact of internal variability on rare events (for examples, see refs. [31,32]). Results also differ among models, as differences in the amount of warming and in the magnitude of variability combine into an uncertain future risk of exceeding a given threshold (Fig. 3b). Validating not only a model's climatology or mean trend but also its variability thus emerges again as an important step when investigating, and ultimately constraining, future projections in this case of extreme events[41].

Attribution-focused LEs differ from those in the MMLEA in that they often rely on regional or high-resolution global atmosphere–land models to capture the small spatial scales of specific extreme

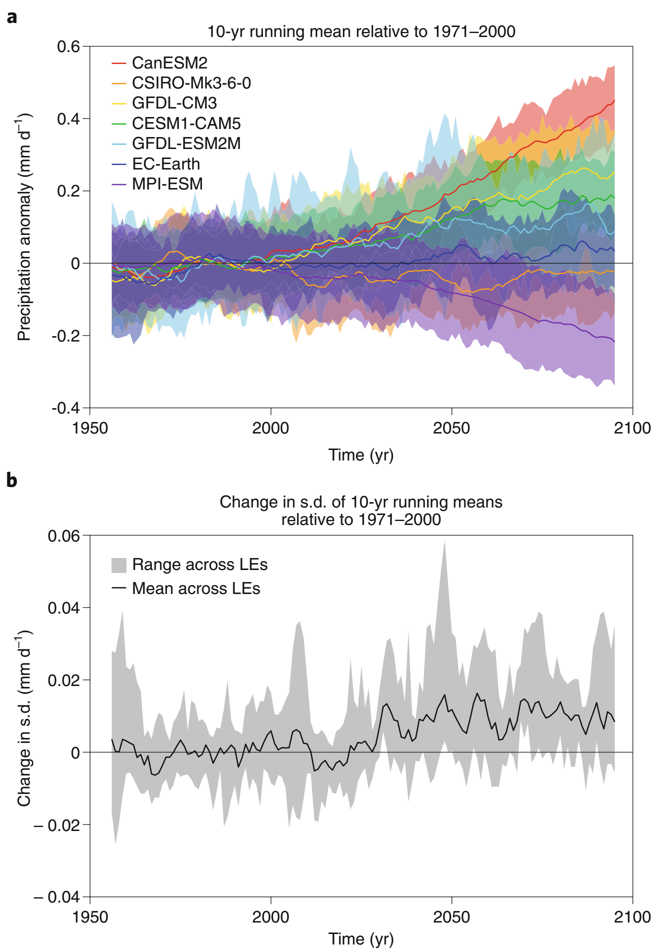

Fig. 2 | Decision-making under uncertainty: changes in mean and variability. a, 10-yr running mean annual precipitation anomalies (mm d^{-1}) over the Upper Colorado River Basin (approximated as a spatial average over 38.75–41.25° N and 111.25–106.25° W) relative to the reference period 1971–2000 from each of the seven model LEs. Solid lines show the ensemble means, and colour shading the 5–95% range across ensemble members. **b**, Moving average of the change in standard deviation of 10-yr mean precipitation (relative to 1971–2000), calculated across the individual ensemble members of each model LE. The thick black curve shows the mean, and grey shading shows the 5–95% range across the seven models. Note the order-of-magnitude smaller range in the *y* axis in **b** compared to **a**. s.d., standard deviation.

events[35–37,42,43], and may prescribe additional boundary conditions, such as the large-scale atmospheric circulation[44,45]. Nevertheless, these types of ensembles highlight the large number of simulations required to identify significant shifts in the probability of certain events. We note that LEs can also serve these alternate types of ensembles by providing lateral boundary conditions to more specialized regional climate models[46] and oceanic boundary conditions to higher-resolution global atmosphere–land models.

Multi-model LEs as methodological testbeds for observations

Another key usage of LEs is to test methods suitable for application to the observational record, for example those aimed at separating the signals of internal variability and forced climate change from a single realization (for examples, see refs. [29,30,47–51]). Using observations alone, it is difficult to assess the skill of such separation methods due to lack of true knowledge of the observed forced response or the full range of variability, including extremes. However, separation methods can be evaluated by applying the methodology to each LE member individually and comparing the results to the model's forced response, estimated from the ensemble mean of the LE (Fig. 4). Application to the MMLEA will identify if the validation has a strong dependence on model structure.

An additional testbed application of model LEs is the development of surrogate realizations of internal variability based on observations (Fig. 4). Although one cannot replay the 'tape of history'[52] with an initial-condition perturbation in the real world, the single observed trajectory is only one of many that could have plausibly occurred (under the same boundary conditions and forcing). The underlying premise of LEs is that internal variability can unfold with a different (and largely unpredictable) chronology, creating uncertainty in the estimate of trends that are calculated over a finite time interval. Can the sample of internal variability in the observational record be used to generate surrogate realizations whose statistical characteristics are largely unchanged, but whose temporal sequences are altered? If so, an observationally based LE can be developed, wherein these surrogates are added to an estimate of the forced response (derived from models or empirical methods applied to observations) to produce an observationally constrained range of outcomes (Fig. 4).

Several methods for generating surrogate realizations that aim to preserve the temporal[26] and spatio-temporal characteristics of observed internal variability have been proposed[47,53–59]. To date, these techniques have been applied to terrestrial temperature and precipitation[26,47,59], sea level pressure[47] and sea-surface temperature[53,55]. These methods interact in two important ways with model LEs. First, model LEs can be used as methodological testbeds to ensure that the statistical ensembles have the desired properties (Fig. 4). Second, after the statistical ensembles are validated, they can then be used to validate the model LEs. We demonstrate this interplay with an example from the Observational Large Ensemble (Obs-LE) developed by ref. [47] (see Methods).

Analogous to the approach mentioned above for estimating the forced trend, the Obs-LE methodology can be tested in the context of a model LE by creating a statistical ensemble based on a single member of the model LE, and assessing whether the spread of the statistical ensemble is consistent with that of the remaining ensemble members. This procedure can then be repeated for each ensemble member, and the resulting information pooled for a robust estimate of the accuracy of the methodology (Fig. 4). In the case of annual temperature trend variability over the past 50 years on land, the fractional error of the Obs-LE methodology is generally less than 20% over most of the globe, with slightly larger errors in certain regions of the tropics (Fig. 5a). Assuming the properties of the real world are not drastically different from those of the model, this indicates that applying the same approach to generate a statistical ensemble from the single realization of the real world is valid.

Having validated the Obs-LE approach, one can then assess the realism of internal variability simulated by each model LE by comparison with the Obs-LE. Regarding the CESM1-LE case, the model overestimates variability of 50-year temperature trends by up to 50% in parts of western North America and northern Eurasia, and up to 100% in areas of high terrain in the tropics (Fig. 5b). These model biases are larger than the error of the Obs-LE methodology, indicating they are true model biases. Similar results are found for precipitation trend variability, which exhibits regions of both significant underestimation and overestimation in the CESM1-LE[47].

One can also apply the Obs-LE to evaluate the simulated distributions of temperature trends at specific locations. For example, the simulated temperature trend distribution for Dallas, Texas, in the CESM1 and LE narrows considerably when the Obs-LE is used to estimate the internal variability (Fig. 5b), which is consistent with the model's significant overestimation of variability at this location.

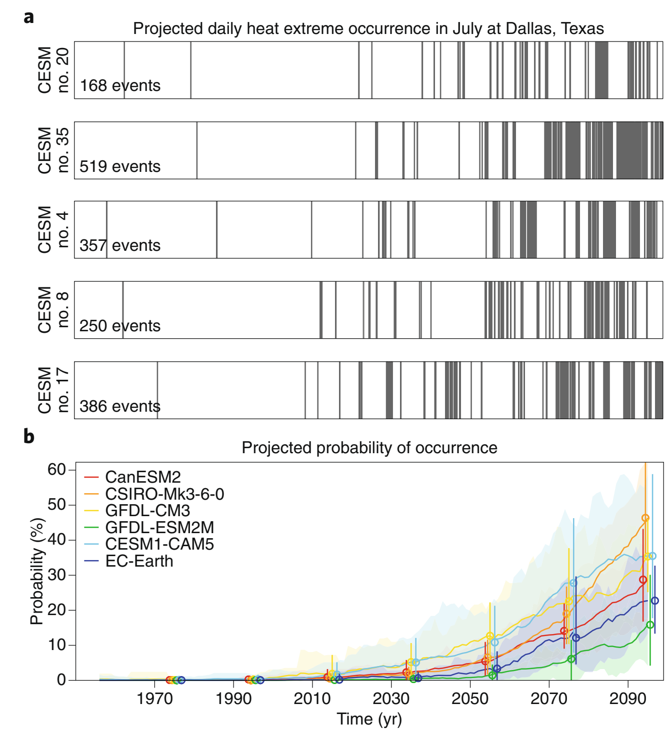

Fig. 3 | Decision-making under uncertainty: changes in extremes. **a**, Vertical bars mark the occurrence of July days that meet or exceed the historical (1950–1999) 99.9th temperature percentile for the grid box containing Dallas, Texas, in five members of the CESM1-LE under historical and future (RCP 8.5) radiative forcing. The 99.9th percentile is defined as the average of the 99.9th percentile values calculated for each ensemble member. **b**, Probability of exceeding the historical (1950–1999) 99.9th percentile of daily temperature in July at Dallas, Texas, for six model LEs. Thick coloured lines show the probability in each LE calculated over all ensemble members, and colour shading shows the 5–95th percentile range based on calculating the probability in each ensemble member separately. Open circles and vertical bars show those same values for every other decade from 1970 onwards, with models plotted in a staggered fashion centred on year five of a given decade.

This brings the observed trend closer to the lower tail of the distribution. It is worth emphasizing that without an observationally based LE, it would not have been possible to assess the width of the models' temperature trend distributions, which indicate important implications for constraining future projections.

An important future challenge for the LE community is to develop effective means to evaluate and benchmark the internal variability generated by model LEs. Meeting this challenge requires taking advantage of historical and paleoclimate records, and developing suitable statistical emulation methods to construct observationally based LEs for other components of the climate system. Statistical emulation of internal variability may also be advantageous in the context of ESMs when the cost of conducting a sufficiently large LE is prohibitive; for example, in the case of models with increased spatial resolution and/or complexity (discussed further below in the sub-section titled 'Designing future initial-condition LEs'). These statistical emulation methods will need to take into account any projected changes in internal variability[60].

Designing future initial-condition LEs

The existing LEs have been designed and created independently, with different choices of time period, radiative forcing scenario, number of members and method of initialization (Table 1). In addition, they employ different protocols for data output, storage and access. These differences must be considered when comparing LEs across models, as each has ramifications.

Initialization. In some LEs, the initial conditions are created by introducing miniscule perturbations (at the level of round-off error or 10^{-14} K, also known as 'micro perturbation'[15]) into the atmosphere. The rapid growth of atmospheric perturbations makes this technique well suited for studies involving atmospheric variability and trends. However, for persistent phenomena involving oceanic or terrestrial processes, it may be more desirable to start each member from completely different initial conditions in the ocean and other components (also known as 'macro perturbations') to better sample possible climate trajectories. Macro perturbations can increase ensemble utility but also introduce subsurface ocean drift in the control simulation that can influence ocean initial conditions; thus, they require long and quasi-equilibrated control simulations to choose initial conditions from[61]. A combination of micro and macro perturbations could have the most scientific benefit, but ensemble initialization procedures need close examination and potential coordination among LE projects.

Length of simulation and ensemble size. For a given amount of computer time, there is a trade-off between the number of ensemble members and their length. For example, is it better (for some purposes) to have a 100-member ensemble covering the period 1981–2040, or a 50-member ensemble extending over 1981–2100? Furthermore, if higher spatial resolution is critical, such as for the simulation of some climate extremes, this usually comes at the expense of the total number of ensemble members that can be run. The optimal balance between ensemble size and spatial resolution will depend on the LE application (for further details, see ref. [62]).

Radiative forcing scenario. The forcing scenario may impact the characteristics of internal variability. Is it better to run more members using a single choice of a forcing scenario, or multiple smaller ensembles with differing scenarios? Even single scenarios are normally comprised of individual forcing components (for example, greenhouse gases and aerosols), and for the important but otherwise elusive goal of attribution, the use of ensembles with a single radiative forcing (for example, only changing aerosols) can provide critical insight into the mechanistic drivers[63,64].

Data output, storage and access. As the LE applications expand to broader timescales (diurnal to centuries), practical limitations arise from the computational burden and storage requirements of maintaining hundreds of terabytes of data for analysis. At present, some LEs only provide monthly averaged output, while others provide daily averages but only for select fields. In general, practical storage limitations require a compromise between ensemble size and choice of output fields. Model fields can also be in non-intuitive formats for users, limiting accessibility. Careful consideration should be given not only to data storage, enabling workflows that bring analysis to the data, but also to format. We recommend single-variable time series. We also encourage modelling centres to provide some LE output interpolated onto conventional grid structures and/or tools to accomplish this re-gridding—for example, for non-uniform ocean model output.

Accommodating increases in model complexity and resolution

High-resolution regional climate projections can also benefit from MMLEs. As mentioned above, statistical and dynamical downscaling techniques can help resolve processes at smaller spatial scales. Such efforts are currently limited by the trade-off between ensemble

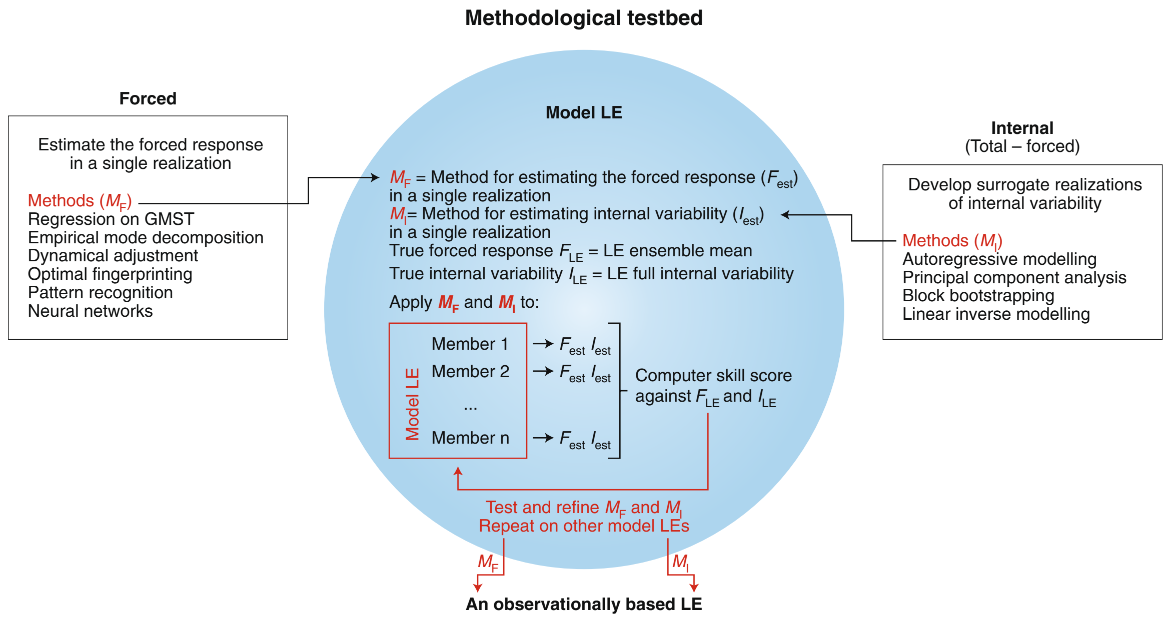

Fig. 4 | Schematic showing the how model LEs can be used to test methods suitable for application to the single observational record; for example, those aimed at separating forced climate change from internal variability. A method (M_F) for estimating the forced response (F_{est}) can be validated using a model LE by applying it to each ensemble member individually and comparing the results to the model ensemble mean (F_{LE}) using a skill score. Similarly, a method (M_I) for developing surrogate realizations of internal variability (I_{est}) can be validated using a model LE by applying it to each ensemble member individually and comparing the results to the full range of internal variability across the model LE (I_{LE}). Various methods (M_F and M_I) are listed (see text for references). After validating the methods, they can be applied to the observational record to construct an observationally-based LE (see main text for details).

size and spatial resolution, with most studies performing downscaling from only one LE and for only part of the globe (for examples, see refs. [46,65]). An alternative approach is to select events of interest from a MMLE, such as particular extremes (for example, see ref. [66]) or El Niño–Southern Oscillation (ENSO) events (for examples, see refs. [67,68]), and perform regional downscaling to understand their dynamics and predictability. Finally, we note that other ensemble methodologies could benefit from incorporating the information from initial-condition LEs into their design. For example, perturbed parameter ensembles[69] can be a useful approach to probe the uncertainties arising from the lack of constraint on uncertain model parameters. However, they will only serve their purpose if, for each parameter combination, a sufficient number of ensemble members exists to allow for the isolation of that parameter influence amidst internal variability.

Despite the added value by multiple-ESM LEs, the ever-growing need for higher spatial resolution[70] and more comprehensive representations of the Earth system poses an enormous computational challenge, especially balanced against other demands for resources in the use and continued development of climate models, such as refining spatial resolution, improving numerical methods, incorporating more realistic and comprehensive physical and biophysical processes, and saving ever-expanding volumes of data.

We see two potential pathways from here: one is the continuation of the current path, creating and extending LEs with the newest models; the second is to focus on developing new techniques that can create efficient statistical descriptions of the complete distribution from LEs, including extreme events[47,56–58]. These emulation techniques would allow the generation of arbitrarily large ensembles at a fraction of the computational cost associated with the traditional LEs, but they would require focused development and validation using existing LEs. If this capability were realized, computational resources could be focused on limited sets of ensembles employing very-high-resolution, comprehensive Earth system models—the types that many applications now demand. After training on the new 'super' data sets produced by these models, the goal is that the new emulation techniques could produce arbitrarily LEs indistinguishable from the training data. One could envision a paradigm in which the required ensemble size for the most comprehensive high-resolution models would be the smallest number that is able to both (1) satisfactorily characterize the model's response to radiative forcing and (2) provide a sufficient data set for training the emulators. A community discussion on how to optimize the scientific return on computational investment from LEs while continuing to advance climate modelling along multiple pathways would be of great value.

Emerging Earth system applications

Several communities have developed approaches to balance the trade-offs between increasing complexity and computational costs. In some cases, raw, bias-corrected or downscaled meteorological fields archived from climate models are used to drive offline models that include more complexity (for example, atmospheric composition, air quality and hydrologic models) or to conduct impact assessments (health burdens, economic valuations and reservoir operations)[71–73]. While these trade-offs will persist as next-generation developments in atmospheric chemistry, hydrology and resource management, and integrated assessment approaches continue to expand in complexity, the development of LEs and MMLEs represents a new research frontier for these applications. Below, we highlight some climate subfields where advances should be possible with the existing climate-focused MMLEs as well as examples where LEs with more complexity are already advancing scientific knowledge (such as ocean biogeochemistry) and where a single LE has yet to be generated (such as atmospheric chemistry). We also discuss LEs' applications across the Earth system.

Several stakeholder communities may be well-positioned to immediately tap into the power of the existing MMLEs. By providing large sample sizes, LEs enable construction of probabilistic frameworks for risk assessment. For example, the existing MMLE

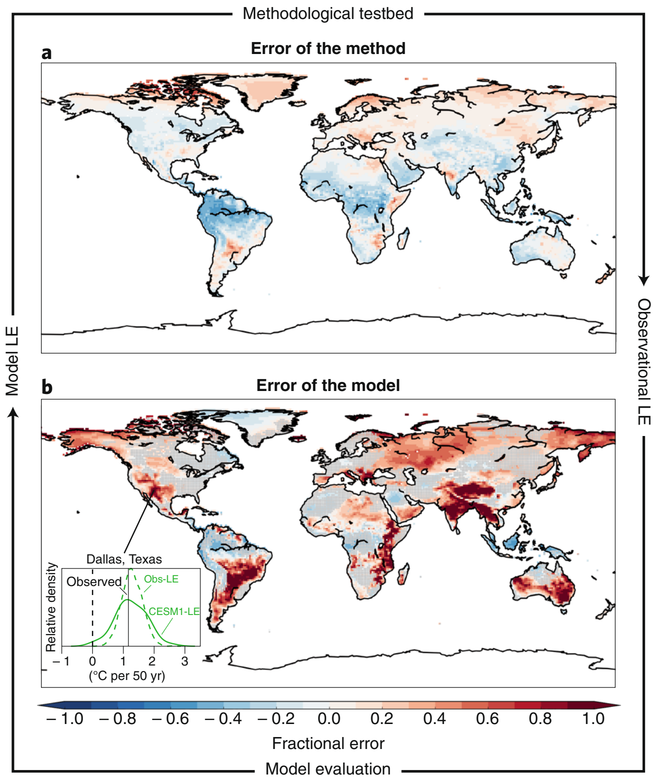

Fig. 5 | Interplay between a Model LE and an Observational LE. The schematic illustrates how a model LE can be used to test the accuracy of a method for deriving surrogate realizations of internal variability based on the observational record to build an observational LE (Obs-LE), and how an observational LE can, in turn, be used to evaluate the model's simulation of internal variability. **a**, The fractional difference between the spread in 50-yr trends of annual near-surface air temperature in the CESM1-LE and the spread estimated from applying the methodology of McKinnon and Deser (ref. [47]) to individual members of the CESM1-LE. **b**, The fractional difference between the spread of 50-yr trends (1965–2014) in CESM1-LE and Obs-LE (areas in grey indicate that the difference is not significant). After McKinnon and Deser (ref. [47]). Inset: probability distribution functions of 50-yr annual temperature trends for the grid box containing Dallas, Texas, from the CESM1-LE (the green solid curve shows the model results; the green dashed curve shows the results based on internal variability from the Obs-LE). The vertical black bar shows the observed 1965–2014 trend value from Berkeley Earth Surface Temperature.

archive may offer opportunities to flesh out the tails of probability distributions of future public health burdens, crop yields or fisheries catch. That is, to the extent that the probabilistic occurrence of complex extreme phenomena can be assessed using commonly simulated meteorological variables (for examples, see refs. [74–76]), a MMLEA offers the ability to independently assess the contributions role of internal variability, anthropogenic climate change and model uncertainty to projected changes. By design, such statistical approaches inherently assume that the key drivers are meteorological and neglect feedback with, for example, the biosphere, that can be included in more specialized ESMs; for example, Coupled Chemistry Models. The power of LEs—even without additional complexity—as tools to investigate mean state biases[77] and extreme events, as well as their impacts on ecosystems, food security and public health, remains largely unexplored.

A growing collection of ocean biogeochemistry studies has highlighted the utility of single-model LEs for quantifying the time of emergence for important biogeochemical variables such as air–sea carbon dioxide fluxes[24], interior ocean oxygen concentration[25], marine ecosystem drivers[78] and interior ocean carbon cycling[79]. Additional work with single-model LEs has been used to quantify the role of internal variability in projection uncertainty for air–sea carbon dioxide fluxes[80] and ecosystem stressors[81] to identify avoidable impacts in the future evolution of phytoplankton net primary production with anthropogenic climate change[82], and to quantify the number of ensemble members needed to detect decadal trends in air–sea CO_2 flux[83]. While changes in phenology under future climate perturbations have been examined in a single LE for a terrestrial ecosystem[84], we anticipate much broader future applications to both terrestrial and oceanic ecosystems, as there are clear implications for ecosystem behaviour and resource management.

Due to the computational expense of simulating atmospheric chemistry within fully coupled ESMs, atmospheric composition and air quality have not yet been explored within a single LE, even though it is well established that atmospheric constituents vary with weather and climate. Changes in pollution events and public health burdens have been investigated through dynamical downscaling (for examples, see refs. [72,85]) of a limited period from global climate models, or directly from coarse resolution global chemistry–climate models (for an example, see ref. [86]). To date, these projections of future composition and air quality have not sufficiently separated internal variability from the forced signal as they rely on small ensembles from a single model (for examples, see refs. [73,87]) or multi-model time-slice ensembles (for examples, see refs. [88,89]). Nevertheless, a small ensemble from one chemistry–climate model demonstrates the need to account for internal variability when detecting future changes in air quality (or, by extension, atmospheric composition) resulting from anthropogenic climate and emission changes[90,91]. A single LE with full atmospheric chemistry would enable pursuit of new research questions paralleling those tackled within the climate community. The future development of MMLEs with full atmospheric chemistry would enable exploration of model structural uncertainty separately from internal variability.

While LEs alone enable one to quantify variations in some variable of interest, in some applications, a set of companion simulations further enhance their utility for decision making. For example, air quality planners would like to understand not just the role of climate change and variability, but also the influence of air pollutant emission pathways on future projections. One path to address this need could be to follow the approach discussed above for extreme events, in which high-frequency time fields are saved for use in dynamical downscaling. Archiving fields needed to drive air quality models would open up the possibility for multiple sensitivity simulations focused on a target time period and region, or even single pollution event, of interest. Another example involves resource managers who are interested in near-term prediction (1–10 year time scales). The CESM-LE, when paired with the CESM Decadal Prediction Large Ensemble, has been shown to provide a significant advance in deepening our understanding of near-term predictability and its origin[92].

Part of the promise offered by LEs is in informing optimization of observing system design and duration. For example, in fields where observations are notoriously sparse (such as ocean biogeochemistry), LEs offer a powerful approach to assess where future measurements can most readily detect trends driven by anthropogenic forcing (for example, where signal-to-noise ratios are greatest). In turn, LEs are useful for interpreting limited observational datasets in the context of internal variability. Internal variability can vary strongly with anthropogenic forcing in nonlinear systems, such as ocean carbonate or atmospheric chemistry; however, without a LE, this signal is challenging to identify. The development of MMLEs in these fields would further allow investigation of model structural uncertainty separately from internal variability.

Fostering effective LE design and incorporation into CMIP7

Enabling discovery for a broad community is key to justifying the resources required for effective LE projects. Designing LE experiments with useful outputs and bringing diverse workflows to these large datasets is challenging. How do we foster effective design and implementation? The experience of this author list in generating and sharing data, including the most widely used LE project to date (the NCAR CESM1-LE Project[19]), provides several lessons. First, open and free access to variables from a range of model components (such as ocean, atmosphere, land and ice) is critical. Involving a broad user community at the outset is essential to identify which variables and temporal frequencies to output as well as to decide on aspects like ensemble size, temporal duration, radiative forcing scenario and method of initialization. Second, data should be distributed in a format that is easily ingested into user workflows. The current gold standard data format is single variable time series in a self-documenting format (for example, NetCDF[93]) on a uniform latitude–longitude grid. Third, well-written documentation that enables users to plan and realize their applications is necessary. As is well known from CMIP and previous LE efforts, documentation and communication about climate modelling projects requires dedicated human resources. Updates must be continuous, easily accessed and responsive to user concerns and questions. While easy-to-use data formats and effective documentation will be enough for experienced users, entraining new and non-traditional users is also needed. Targeted tutorials and example analysis workflows will enable more users to become involved. Finally, it is necessary to consider not only the computational needs for producing LE data, but also the long-term storage and computational requirements to make these data usable, free and accessible over time. Effective user accessibility and data storage will allow researchers to build on the foundation of the original LE to complete off-shoot experiments, something that is only possible if the original code and climate model restart files are maintained and distributed publicly. Future LE projects should also move away from workflows where the burden is on individual users for data download, storage and analysis. The potential of the commercial cloud is worth exploring in this respect while also acknowledging the complications that may arise, like intellectual property rights and monetary costs. Careful thought and resources to address these above four considerations undoubtedly contributed to the widespread use and success of the CESM1-LE and are informing the design of next-generation LEs. Experience shows that choices made in the design and implementation of a LE have substantial implications for its scientific utility.

While LE experiments have witnessed success outside of official CMIP coordination, we recommend increased integration and assessment of LE experiments within CMIP7. Incorporating LE design and knowledge into the next phase of CMIP has the potential to directly address the challenges of partitioning projection uncertainty into structural and internal variability components. For CMIP7, we recommend that modelling centres have a strategy to incorporate quantification of internal climate variability into all of their MIP contributions. Without such a strategy, we are concerned that internal climate variability will, at times, continue to be impossible to differentiate from model uncertainty and/or forcing uncertainty. Moving forward, it is critical that the science and policy communities have the capacity to assess internal variability contributions to climate projections.

Final remarks

Models form much of the scientific basis for future climate change projections. While the scientific and policy communities have focused on multi-model archive CMIP projections, these experiments often confound structural uncertainty (that is, differences in model formulation, including physics, parameterizations, resolution and so on) with internal variability. With the continuously growing MMLE archive introduced here, identifying anthropogenic influences on climate amidst the noise of internal variability from a multi-model perspective is finally possible. Scrutiny of this newly available MMLE archive is needed, as are answers to the question 'is a model's internal variability realistic?'. Separating signal from noise is a grand challenge for all areas of climate science, and one that spans all components of the Earth system. Pairing the long-term statistics of the internally driven noise of the climate system provided by LEs with, for example, high-resolution simulations, suggests a viable path forward to improve understanding of both the statistics and processes underlying extremes. Looking forward, a broad community from computational scientists to stakeholders must be engaged to maximize scientific return on the computing and human investment in new LE efforts.

Online content

Any methods, additional references, Nature Research reporting summaries, source data, extended data, supplementary information, acknowledgements, peer review information; details of author contributions and competing interests; and statements of data and code availability are available at https://doi.org/10.1038/s41558-020-0731-2.

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Methods

Calculations for Fig. 1. Trends in annual mean temperature over 1951–2010 are calculated as an ordinary least squares linear fit at each grid cell. The probability distribution functions (PDFs) show the trend in spatially averaged temperature. Distributions are computed by fitting a kernel density estimate (using Matlab's 'ksdensity') to the histograms of trends from each LE and from CMIP5. From CMIP5, a set of available model simulations with historical and RCP 8.5 forcing were used, ranging between 1 and 11 ensemble members per model, totalling 123 simulations. Observations are from the Berkeley Earth Surface Temperature data set[61].

The Obs-LE. A brief description of the method used to construct Obs-LE is given here; further details are available in ref. [47]. The Obs-LE provides surrogate realizations of internal variability that could have happened in the real world while largely preserving the full spatio-temporal characteristics of the actual observational record. Internal variability in the Obs-LE is the sum of two pieces: a component that captures variability linearly related to the three dominant ocean-atmosphere modes in the climate system (ENSO, the Pacific Decadal Oscillation[99] and the Atlantic Multidecadal Oscillation[100]), and a component termed residual 'climate noise', which primarily emerges from unpredictable atmospheric variability. Both pieces are estimated using monthly mean temperatures from Berkeley Earth Surface Temperature (BEST) over the period 1920–2015 after an empirical removal of the forced trend following ref. [101]. The spread across the ensemble is a result of the inherent randomness of both the mode time series and the residual climate noise; both components contribute approximately equally to the spread, although one may be more dominant than another in a given location (see Fig. 8 in ref. [47]). The mode component is computed first and then subtracted from the total internal variability to obtain the residual component. Specifically, the Obs-LE is created through: (1) generating new time series of the three modes that share the same autocorrelation and distributions as the observed ones but have different temporal phasing, and multiplying them by the spatial pattern of temperature sensitivity to each mode; and (2) applying a two-year block bootstrap in time to the residual climate noise component. The choice of a two-year block to perform the bootstrapping provides a suitable balance between accommodating any remaining temporal autocorrelation in the residual noise component and number of independent samples in the record. The approach makes a key assumption that the internal variability (including teleconnection patterns) of monthly temperature has not changed over the period used to fit the model, and, if used for projections, will not change in the future period.

Data availability

All data used in this study are publicly available. The CMIP5 simulations are available through PCMDI, the large ensembles are available at the MMLE Archive and the observational data are available through the respective institutions.

Code availability

Code to produce Figs. 1–3 can be obtained from F.L.

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Author contributions

C.D., F.L. and K.R. conceived the study. C.D., F.L. and K.A.M. performed the analysis and created the figures. C.D. and F.L. led the writing of the manuscript, with contributions from all authors. C.D. and F.L. contributed equally to the work.

Competing interests

The authors declare no competing interests.

Additional information

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