



Towards neural Earth system modelling by integrating artificial intelligence in Earth system science

Christopher Irrgang¹✉, Niklas Boers^{2,3,4}, Maike Sonnewald^{5,6,7}, Elizabeth A. Barnes⁸, Christopher Kadow⁹, Joanna Staneva¹⁰ and Jan Saynisch-Wagner¹

Earth system models (ESMs) are our main tools for quantifying the physical state of the Earth and predicting how it might change in the future under ongoing anthropogenic forcing. In recent years, however, artificial intelligence (AI) methods have been increasingly used to augment or even replace classical ESM tasks, raising hopes that AI could solve some of the grand challenges of climate science. In this Perspective we survey the recent achievements and limitations of both process-based models and AI in Earth system and climate research, and propose a methodological transformation in which deep neural networks and ESMs are dismantled as individual approaches and reassembled as learning, self-validating and interpretable ESM-network hybrids. Following this path, we coin the term neural Earth system modelling. We examine the concurrent potential and pitfalls of neural Earth system modelling and discuss the open question of whether AI can bolster ESMs or even ultimately render them obsolete.

For decades, scientists have used mathematical equations to describe geophysical and climate processes and to construct deterministic computer simulations that allow for the analysis of such processes. Until recently, process-based models had been considered irreplaceable tools that helped us to understand the complex interactions in the coupled Earth system and provided the only tools with which to predict the Earth system's response to anthropogenic climate change.

Earth system models (ESMs)¹ combine process-based models of the different subsystems of the Earth system into an integrated numerical model that for a given state of the coupled system at time t yields a prediction of the system state for time $t + 1$. The individual model components, or modules, describe subsystems including the atmosphere, the oceans, the carbon cycle and other biogeochemical cycles, and radiation processes, as well as land surface and vegetation processes and marine ecosystems. These modules are then combined by a dynamic coupler to obtain a consistent state of the full system for each time step.

The inclusion of a vastly increasing number of processes, together with continuously rising spatial resolution, have led to the development of comprehensive ESMs to analyse and predict the state of the Earth system. From the First Assessment Report of the Intergovernmental Panel on Climate Change (IPCC) in 1990 to the Fifth Phase of the Climate Model Intercomparison Project (CMIP5)² and the associated Fifth Assessment Report of the IPCC in 2014, the spatial resolution has increased from around 500 km to as high as 70 km. In accordance, the CMIP results show that over the course of two decades the models have greatly improved in their accuracy in reproducing crucial characteristics of the Earth system, such as the evolution of global mean temperatures since instrumental data became available in the second

half of the nineteenth century, or the average present-day spatial distribution of temperature or precipitation^{3,4}.

The provocative thought that ESMs might lose their fundamental importance in the advent of novel artificial intelligence (AI) tools has sparked both a gold-rush feeling and caution in scientific communities. On the one hand, deep neural networks have been developed that complement and aim to match the skill of process-based models in various applications, ranging from numerical weather prediction to climate research. On the other hand, most neural networks are trained for isolated applications under simplified conditions and lack true process knowledge. Regardless, the daily increasing data streams from Earth system observations (ESOs), increasing computational resources, and the availability and accessibility of powerful AI tools—particularly in machine learning (ML)—have led to numerous innovative developments that aim to resolve persistent shortcomings of current ESMs.

In the following, we survey the current state, recent achievements and recognized limitations of both process-based modelling and AI in Earth and climate research. On the basis of this survey, we draw an overview of an imminent and profound methodological transformation, hereafter named neural Earth system modelling (NESYM), that aims for a deep and interpretable integration of AI into Earth system modelling. We discuss emerging challenges of this approach and highlight the necessity of new transdisciplinary collaborations between the involved communities.

Overview of Earth system modelling and ESOs

For some parts of the Earth system, the primitive physical equations of motion are known explicitly, such as the Navier–Stokes equations that describe the fluid dynamics of the atmosphere and oceans

¹Helmholtz Centre Potsdam, German Research Centre for Geosciences GFZ, Potsdam, Germany. ²Department of Mathematics and Computer Science, Free University of Berlin, Berlin, Germany. ³Potsdam Institute for Climate Impact Research, Potsdam, Germany. ⁴Department of Mathematics and Global Systems Institute, University of Exeter, Exeter, UK. ⁵Program in Atmospheric and Oceanic Sciences, Princeton University, Princeton, NJ, USA. ⁶Ocean and Cryosphere Division, Geophysical Fluid Dynamics Laboratory, NOAA/OAR, Princeton, NJ, USA. ⁷School of Oceanography, University of Washington, Seattle, WA, USA. ⁸Colorado State University, Fort Collins, CO, USA. ⁹German Climate Computing Center DKRZ, Hamburg, Germany. ¹⁰Institute of Coastal Systems, Helmholtz-Zentrum Hereon, Geesthacht, Germany. ✉e-mail: irrgang@gfz-potsdam.de

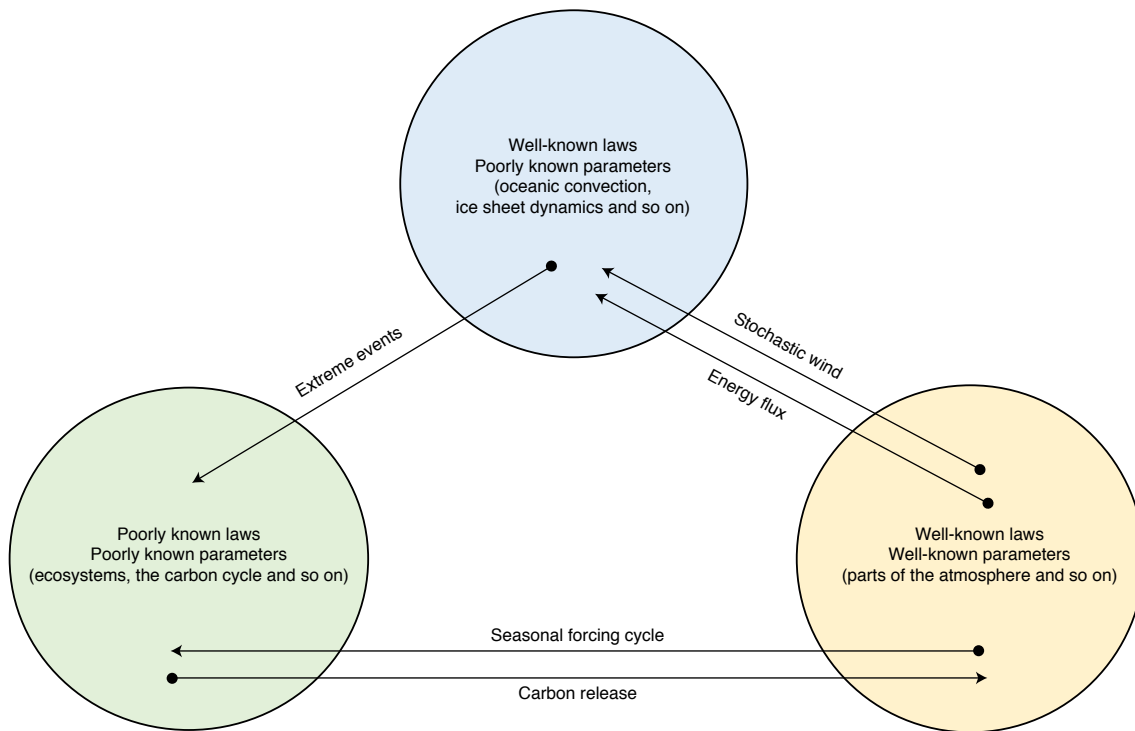


Fig. 1 | Symbolic representation of Earth system components in terms of knowledge clusters. Arrows indicate exemplary exchange of information between the clusters in terms of geophysical processes and coupling mechanisms. ML can take over different tasks depending on the cluster application; for example, data exploration and analysis in case of poor process knowledge (green cluster), ESM enhancement by improving insufficient parameterizations and other simplifications in process-based models (blue cluster) or emulation and acceleration of well-understood process-based simulations (orange cluster). Similarly, ML can be applied to coupling mechanisms and interaction processes (arrows), utilizing adjacent clusters as training data pools.

(Fig. 1). In practice, it is impossible to numerically resolve all relevant scales of the dynamics and approximations have to be made. For example, the fluid dynamical equations for the atmosphere and oceans are integrated on discrete spatial grids, and all processes that operate below the grid resolution have to be parameterized to assure a closed description of the system. Since the multiscale nature of the dynamics of geophysical fluids implies that the sub-grid-scale processes interact with the larger scales that are resolved by the model, (stochastic) parameterization of sub-grid-scale processes is a highly non-trivial, yet unavoidable, part of climate modelling^{5–7}.

For other parts of the Earth system, primitive equations of motion, such as the Navier–Stokes equations, do not exist. Essentially, this is due to the complexity of the Earth system, in which many phenomena that emerge at a macroscopic level are not easily deducible from microscopic scales that may or may not be well understood. A typical example is given by ecosystems and the physiological processes governing the vegetation that covers vast parts of the land surface, as well as their interactions with the atmosphere, the carbon cycle and other geochemical cycles. Approximations in terms of parameterizations of potentially crucial processes must also be made for these cases.

Regardless of the specific process, such parameterizations induce free parameters in ESMs for which suitable values have to be found empirically. The size of state-of-the-art ESMs mostly prohibits systematic calibration methods such as, for example, the ones based on Bayesian inference, and the models are therefore often tuned manually. The quality of the calibration, as well as the overall accuracy of the model, can only be assessed with respect to relatively sparse observations of the last 170 years, at most, and there is no way to assess the models' skill in predicting future climate conditions⁸.

Although necessary, parameterizations can cause biases or structural model errors. The example of the discretized spatial grid suggests that the higher the spatial resolution of an ESM, the smaller the potential errors. Likewise, it is expected that the models' representation of the Earth system will become more accurate the more processes are resolved explicitly.

Despite the tremendous success of ESMs, persistent problems and uncertainties remain:

1. A crucial quantity for the evaluation of ESMs is the equilibrium climate sensitivity, defined as the amount of equilibrium global mean temperature increase that results from an instantaneous doubling of atmospheric CO₂ (ref.⁹). There remains a large equilibrium climate sensitivity range in current ESMs. From CMIP5 to CMIP6, the likely equilibrium climate sensitivity range has widened from 2.1–4.7°C to 1.8–5.6°C (refs.^{10,11}). Reducing these uncertainties, and hence the uncertainties of future climate projections, is one of the key challenges in the development of ESMs.
2. Both theoretical considerations and palaeoclimate data suggest that several subsystems of the Earth system can abruptly change their state in response to gradual changes in forcing^{12,13}. There is concern that current ESMs will not be capable of predicting future abrupt climate changes, because the instrumental era of less than two centuries has not experienced comparable transitions, and model validation against palaeoclimate data for such events remains impossible due to the length of the relevant timescales¹⁴. In an extensive search, many relatively abrupt transitions have been identified in future projections of CMIP5 models¹⁵, but due to the nature of these rare, high-risk events, the accuracy of ESMs in predicting them remains untested.

3. Current ESMs are not yet suitable for assessing the efficacy or the environmental impact of CO₂ removal techniques, which are considered key mitigation options in pathways realizing the Paris Agreement¹⁶. Furthermore, ESMs are unable to adequately represent key environmental processes such as the carbon cycle, water and nutrient availability or interactions between land use and climate. This can impact the usefulness of land-based mitigation options that rely on actions such as biomass energy with carbon capture and storage or nature-based climate solutions^{17,18}.
4. The distributions of time series encoding Earth system dynamics typically exhibit heavy tails. Extreme events such as heat waves and droughts—and extreme precipitation events and associated floods—have always caused tremendous socio-economic damage. With ongoing anthropogenic climate change, such events are projected to become even more severe, and the attribution of extremes poses another outstanding challenge in Earth system science¹⁹. Although current ESMs are very skilful in predicting average values of climatic quantities, there remains room for improvement in representing extremes.

In addition to the possible solutions to these fundamental challenges, improvements of the overall accuracy of ESMs can be expected from more extensive and more systematic integration of the process-based numerical models with observational data. ESOs are central to ESMs, serving a multitude of purposes; they are used to evaluate and compare process-based model performance, to generate model parameters and initial model states or as boundary forcings of ESMs^{20,21}. ESOs are also used to directly influence the model output by either tuning or nudging parameters that describe unmodelled processes, or by the more sophisticated methods of data assimilation that alter the model's state variables to bring the model output in better agreement with the observations²². Gradient-based optimization, as in four-dimensional variational schemes, is the current state of the art for efficiency and accuracy, but requires time-consuming design and implementation of adjoint calculation routines tailored to each model. Ensemble-based Kalman filter schemes are gradient-free but produce unphysical outputs and rely on strong statistical assumptions that are often unsatisfied, leading to biases and overconfident predictions²³. The main problems of contemporary ESM data assimilation are (1) nonlinear dynamics and non-Gaussian error budgets in combination with the high dimensionality of many ESM components^{24–26} and (2) selecting appropriate constraints on the governing processes over the different spatiotemporal scales found in coupled systems^{27,28}.

ESO cover a wide range of spatiotemporal scales and types, ranging from a couple of centimetres to tens of thousands of kilometres, and from seconds and decades to millennia. The types of observation range from in situ measurements of irregular times and spaces to global satellite-based data fields. Yet, the available observational data pool still contains large gaps in time and space that prevent a holistic observation-driven picture of the coupled Earth system being built as a result of insufficient data resolution, too short observation time periods and largely unobserved compartments of Earth systems such as the abyssal oceans. The combination of these complex characteristics renders ESOs both challenging and particularly interesting for AI applications.

From ML-based data exploration towards learning physics

In contrast to other research branches^{29–32}, the usage of ML in Earth and climate sciences is still in its infancy. Whereas current ML applications are mostly found in explorative studies and are still far away from operational usage, profound impact on research as well as on the supercomputing industry is expected³³. A key observation is that ML concepts from computer vision and automated image analysis can be isomorphically transferred to ESO imagery

and time series^{34,35}. Pioneering studies demonstrated the feasibility of ML for remote sensing data analysis, classification tasks and parameter inversion as early as the 1990s^{36–39}, and climate-model emulation in the early 2000s⁴⁰. The figurative Cambrian explosion of AI techniques in Earth and climate sciences, however, only began in the past 5 years and will rapidly continue throughout the coming decades.

ML has been applied across various spatial and temporal scales, ranging from short-term regional weather prediction to Earth-spanning climate phenomena. Considerable progress has been made in developing purely data-driven weather prediction networks, aiming to explore alternative approaches to process-based model forecasts^{41–43} or to emulate and accelerate computationally demanding components of weather forecasting systems such as the parameterization of gravity wave drag⁴⁴ and the simulation of cloud processes⁴⁵. However, current global data-driven ML weather forecasts operate on much lower resolutions than state-of-the-art process-based models⁴⁶ and the lack of available training data will probably prevent a closure of this gap in the near future⁴⁷. Yet, ML for emulation and acceleration tasks could play an even more important role in this context (orange knowledge cluster in Fig. 1), particularly during the advent of exascale computing⁴⁸ and when the related computational challenges and bottlenecks are addressed⁴⁹. ML contributed to the pressing need to improve the predictability of natural hazards, for instance, by uncovering global extreme-rainfall teleconnections⁵⁰ and by improving long-term forecasts of the El Niño/Southern Oscillation^{51,52}. ML-based image filling techniques were used to reconstruct missing climate information, allowing previous global temperature records to be corrected⁵³. Furthermore, ML was applied to analyse climate data sets to extract specific forced signals from natural climate variability^{54,55}, for example, or to predict clustered weather patterns⁵⁶. In these applications, the ML tools function as highly specialized agents that help to uncover and categorize patterns in an automated way, which is particularly useful for observable processes that are only poorly described through physical laws or parameterizations (green knowledge cluster in Fig. 1). A key methodological advantage of ML in comparison with covariance-based spatial analysis lies in the possibility of mapping nonlinear processes^{57,58}. At the same time, such trained neural networks lack actual physical process knowledge, as they solely function through identifying and generalizing statistical relations by minimizing predefined loss measures for a specific task⁵⁹. Consequently, research on ML in Earth and climate science differs fundamentally from the previously described efforts of advancing ESMs in terms of methodological development and applicability.

Concepts of using ML not only for physics-blind data analyses but also as surrogates and methodological extensions for ESMs have only recently started to take shape⁶⁰. Scientists started pursuing the aim of ML methods learning aspects of Earth and climate physics, or at least plausibly relating cause and effect. The combination of ML with process-based modelling is the essential distinction from previous ESO data exploration (blue knowledge cluster in Fig. 1). Lifting ML from purely diagnosis-driven usage towards the prediction of geophysical processes will also be crucial to aid in climate change research and the development of mitigation strategies⁶¹.

Following this reasoning, ML methods can be trained with process-based model data to inherit a specific geophysical causation or even emulate and accelerate entire forward simulations. For instance, ML has been used in combination with ESMs and ESOs to invert space-borne oceanic magnetic field observations to determine the global ocean heat content⁶². Similarly, a neural network has been trained with a continental hydrology model to recover high-resolution terrestrial water storage from satellite gravimetry⁶³. ML plays an important role in upscaling unevenly distributed carbon flux measurements to improve global carbon monitoring systems⁶⁴. The eddy covariance technique was combined with ML to

measure the net ecosystem exchange of CO₂ between ecosystems and the atmosphere, offering a unique opportunity to study ecosystem responses to climate change⁶⁵. ML has successfully been applied in representing sub-grid-scale processes and other parameterizations of ESMs, providing that sufficient training data were available. As such, neural networks were applied to approximate turbulent processes in ocean models⁶⁶ and atmospheric sub-grid processes in climate models⁶⁷. Here, substantial computational savings could be achieved^{44,45}, freeing up resources that in turn could be used to improve the model simulations, for example, by raising ensemble sizes or improve the resolution of the numerical model. Several studies highlight the potential for ML-based parameterization schemes^{68–72}, helping step-by-step to gradually remove numerical and human-induced simplifications and other biases of ESMs⁷³. Nevertheless, most ML parameterization schemes are still applied under idealized conditions such as coarse model resolution, simplified physics or reduced prognostic model variables. Transferring and testing these achievements on more complex ESM configurations remains an ongoing and open challenge⁷⁴.

Although some well-trained ML tools and simple hybrids have shown higher predictive power than traditional process-based models, only the surface of new possibilities, but also of new scientific challenges, has been scratched. So far, ML, ESMs and ESO have largely been independent tools. Yet, we have reached the understanding that applications of physics-aware ML and model–network hybrids offer huge benefits by filling up niches where purely process-based models persistently lack reliability⁷⁵.

Fusion of process-based models and AI

The idea of hybrids of process-based and ML models is not new⁷⁶, but an understanding of how ML can enhance process-based modelling has evolved following the recent advances. The long-term goal will be to consistently integrate the recently discovered advantages of ML into the already decade-long source of process knowledge in Earth system science (Fig. 2). However, this evolution does not come without methodological caveats, which need to be investigated carefully. For the sake of comparability, we distinguish between weakly coupled NESYM hybrids (in which an ESM or AI technique benefits from information from the respective other) and strongly coupled NESYM hybrids (in which fully coupled model–network combinations dynamically exchange information).

The emergent development of weak hybrids is predominantly driven by the aim of resolving the previously described ESM limitations, particularly unresolved and sub-grid-scale processes (left branch of Fig. 2). Neural networks can emulate such processes after careful training with simulation data from a high-resolution model that resolves the processes of interest, or with relevant ESO data. The next methodological milestone will be the integration of such trained neural networks into ESMs for operational usage. The first tests have indicated that the choice of the AI technique (for example, neural networks versus random forests) seems to be crucial for the implementation of learning parameterization schemes, as they can greatly diminish the ESM's numerical stability⁷⁷. Thus, it is not only important to identify how neural networks can be trained to resolve ESM limitations, but also how such ML-based schemes can be stabilized in the model physics context and how their effect on the process-based simulation can be evaluated and interpreted⁷⁸. The limitations of ML-based parameterization approaches can vary widely for different problems or utilized models and, consequently, should be considered for each learning task individually⁷⁹. Nevertheless, several ideas have been proposed to stabilize ML parameterizations, for example, by enforcing physical consistency through customized loss functions in neural networks and specific network architectures^{71,80} or by optimizing the high-resolution model training data⁷². In addition, an ESM blueprint has been proposed in which learning parameterizations can be targeted through

searching for an optimal fit of statistical measures between ESMs, observations and high-resolution simulations⁸¹. Although this is not strictly applying ML, the approach is well suited to exploring parameterizations suitable for smooth climate solutions, avoiding the problems of the ensemble-based Kalman filter techniques. In such a context, further efforts have been made to enhance an ESM not with ML directly, but in combination with a data assimilation system²². For instance, emulating a Kalman filter scheme with ML has been investigated^{82,83}, an ML-based estimation of atmospheric forcing uncertainties used as error covariance information in data assimilation has been proposed⁸⁴ and ML for nudged hindcasts⁷⁴, as well as further types of Kalman–network hybrid^{85,86}. Despite the demonstrated potential for combining data assimilation and ML, it should be highlighted that many current challenges of data assimilation need to be solved for respective ML approaches as well, such as robust quantification of model and observation uncertainties and the optimal use of sparse observations⁸⁷.

In the second class of weak hybrid, the model and AI tasks are transposed such that the information flow is directed from the model towards the AI tool (right branch of Fig. 2). Here, neural networks are trained directly with model state variables, their trajectories or with more abstract information such as seasonal signals, interannual cycles or coupling mechanisms (knowledge cluster connections in Fig. 1). The goal of the ML application might not only be model emulation but also inverting nonlinear geophysical processes⁶², learning geophysical causation⁸⁸ or predicting extreme events^{89,90}. In addition to these inference and generalization tasks, a key question in this subdiscipline is whether a neural network can learn to outperform the utilized process-based trainer model in terms of physical consistency or predictive power. ESOs play a vital role in this context, as they can serve as additional training constraints for neural network training, allowing the network to build independent self-evaluation measures⁶³.

These examples generally work well for validation and prediction scenarios within the given training data distribution. Out-of-distribution samples, in contrast, pose a huge challenge for supervised learning, which renders the ‘learning from the past’ principle possibly ill-suited to prediction tasks in NESYM. Because of both the naturally and anthropogenically induced non-stationarity of the climate and Earth system, it will be very challenging—and in many cases impossible—for purely data-driven AI methods to perform accurate climate projections on their own. Nevertheless, some hope for purely data-driven AI approaches may remain for problems for which it can be convincingly argued that, for instance, the data distributions for colder-climate training conditions and warmer-climate projections overlap. But in practice it will be hard to guarantee that the unseen domains of the data distributions corresponding to a warmer climate are not relevant for a given process under study. Moreover, in specific cases the scales of the processes under study may to a first approximation be separable from the scales relevant in the context of anthropogenic climate change; guaranteeing this in practice, however, will again be very difficult.

Overcoming the overall limitations posed by the non-stationarity of the climate system requires a deeper holistic integration in terms of strongly coupled hybrids and the consideration of other, less constrained training techniques such as unsupervised training⁹¹ and generative AI methods^{69,92,93}. For example, the problems of pure AI methods with non-stationary training data can be attenuated by combining them with physical equations describing the changing energy balance of the Earth system due to anthropogenic greenhouse-gas emissions⁹⁴. A key distinction of strongly coupled hybrids is that the ML component can be further improved by continued training. As such, the dynamic exchange of information means that the ML part is not only repeatedly called after being trained for usage in a weak hybrid, but can further evolve on the basis of the current model state, newly available observations and

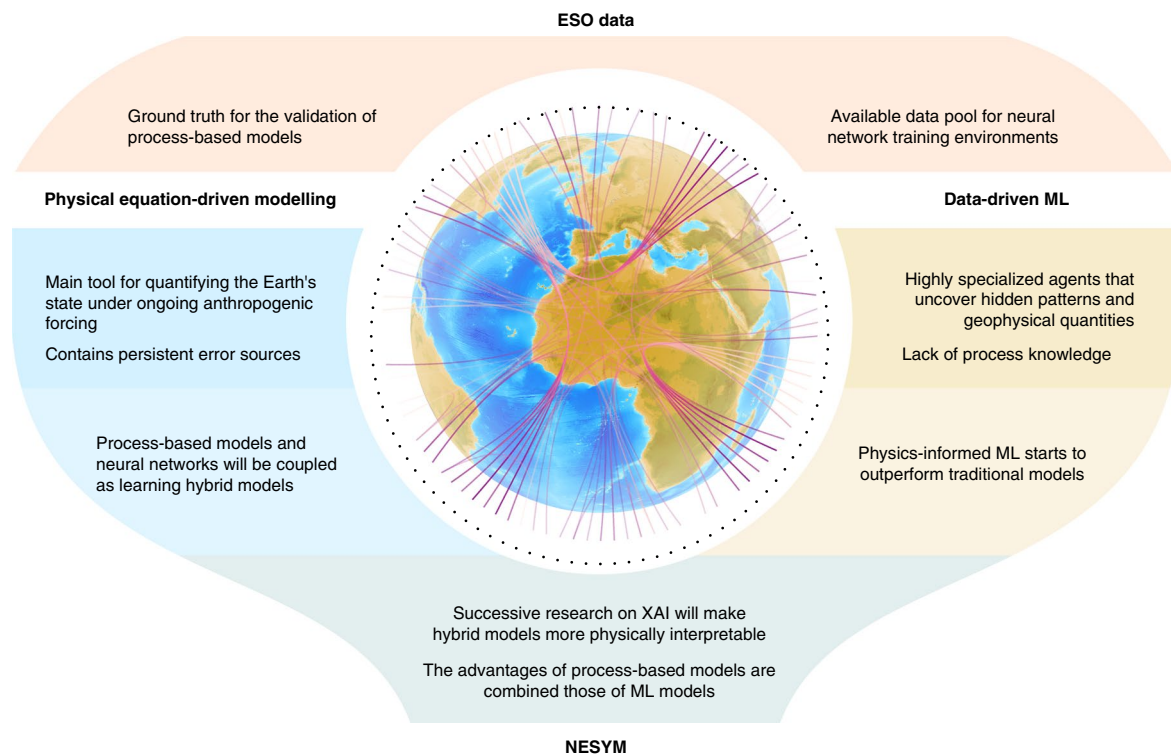


Fig. 2 | Successive stages of the fusion process of ESMs and AI towards NESYM. The left and right branches visualize the current efforts and goals for building weakly coupled hybrids (blue and yellow), which converge towards strongly coupled hybrids with support from XAI. More details of weak and strong hybrids are provided in the text.

so on. In addition, first steps towards physics-informed AI have been made by the ML-based and data-driven discovery of physical equations⁹⁵ and by the implementation of neural partial differential equations^{96,97} in the context of climate modelling⁹⁸.

Continuous development of the methodological fusion process will allow hybrids of neural networks, ESMs and ESOs that dynamically exchange information to be built. ESMs will soon use output from supervised and unsupervised neural networks to optimize their physical consistency and, in turn, feed back improved information content to the ML component. ESOs form another core element and function as the constraining ground truth of the AI-infused process prediction. Similar to the adversarial game of generative networks⁹⁹, or coupling mechanisms in an ESM¹⁰⁰, strongly coupled NESYM hybrids will also require innovative interfaces that control the exchange of information that are as yet unavailable. As the methodical range of weak and strong hybrids is too large to be summarized through a single overarching definition, we formulate key characteristics and define goals of NESYM:

1. Hybrids can reproduce and predict out-of-distribution samples and extreme events
2. Hybrids perform constrained and consistent simulations that obey physical conservation laws despite potential shortcomings of the hybrids' individual components
3. Hybrids include integrated adaptive measures for self-validation and self-correction
4. NESYM allows replicability and interpretability

Whereas most studies implemented neural networks for ML in this context, NESYM includes all AI techniques that help to achieve these goals. The ultimate goal of NESYM is to help scientists improve the current forecast limits of geophysical processes and contribute towards understanding the Earth's susceptible state in a changing climate. Consequently, it is not only the fusion of ESM and

AI that will be a focus of research, but also AI interpretability and the resolution of the common notion of a black box.

Peering into the black box

ML has emerged as a set of methods based on the combination of statistics, applied mathematics and computer science, but it comes with a unique set of hurdles. Peering into the black box and explaining the decision-making process of ML methods, termed explainable AI (XAI), is critical to the use of ML tools. In the physical sciences, adaptation of ML is hampered by a lack of interpretability, particularly of supervised ML. In contrast, and in addition to XAI, there is the call for interpretable AI (IAI)—that is, building specifically interpretable ML models from the beginning, instead of explaining ML predictions through post-process diagnostics¹⁰¹.

Ensuring that what is 'learned' by the machine is physically tractable or causal, and not due to trivial coincidences^{102,103}, is important before ML tools are used, for example, in an ESM setting targeted at decision-making. Thus, interpretability and explainability provides the user with trust in the ML output, improving its transparency. This is critical for the use of ML in the policy-relevant area of climate science, as society is making it increasingly clear that understanding the source of AI predictive skill is of crucial importance^{104,105}. By analysing the decision-making process, climate scientists will be able to better incorporate their own physical knowledge into the ML method, ultimately leading to greater confidence in predictions. Perhaps least appreciated in geoscientific applications thus far is the use of IAI and XAI to discover new science^{103,106} and assist in theoretic advances¹⁰⁷. For example, when an ML model is capable of making skilful predictions, XAI allows us to ask 'what did it learn?'. In this way, ML models can act as investigative tools for discovery.

The power of XAI for climate, ocean and weather applications has very recently been demonstrated^{106,108–110}. Tools for developing XAI models are referred to as additive feature attribution¹¹¹. For

example, neural networks coupled with the XAI attribution method known as layerwise relevance propagation^{112,113} have revealed modes of variability within the climate system, sources of predictability across a range of timescales and indicator patterns of climate change^{55,106}. There is also evidence that XAI methods can be used to evaluate climate models against observations, identifying the most important climate model biases for the specific prediction task¹¹⁴. However, these methods are in their infancy and there is vast room for advancements in their application, making it explicitly appropriate to employ them within the physical sciences^{103,110}. In the context of the above, however, we emphasize that IAI and XAI approaches should go hand-in-hand with well-posed physical research hypotheses. Also in this regard, we again highlight the importance of combining recent methods from AI with domain-specific physical understanding and the state of the art in process-based modelling.

Unsupervised ML can be intuitively IAI through the design of experiments. For example, applying clustering on closed model budgets of momentum ensures all relevant physics are represented, and can be interpreted in terms of the statistically dominant balances between terms¹¹⁵. Similarly, ‘equation driven’ ML can be used to determine the salient terms given an array of mathematical operations, and suggest interpretable sub-grid-scale parameterization developments on this basis^{56,95}. In this manner, dominant physical mechanisms or equation terms can be determined, generating new knowledge in physics and beyond^{91,115,116}. Knowledge of dominant regimes can subsequently be used to engineer features for a well-posed XAI application where the source of predictive ML skill is transparent¹¹⁰. Adversarial learning has been an effective tool for generating super-resolution fields of atmospheric variables in climate models⁹³. Furthermore, unsupervised ML approaches have been proposed for discovering and quantifying causal interdependencies and dynamical links inside a system, such as the Earth’s climate^{88,117}. Another example of an ML application that can be termed IAI is equation discovery, for example using relevance vector machines, which has been applied for ocean eddy parameterizations⁹⁵. It is also worth noting that a revolution of analysis tools has been called for to evaluate climate models, and ML is poised to be part of this change^{60,118,119}.

Given the importance of both explainability and interpretability for improving ML generalization and scientific discovery, promoting collaborations between climate and AI scientists can help to develop methods that are tailored to the field’s needs. This is not just an interesting exercise—it is essential for the proper use of AI for the development and use of NESYM. Earth and climate scientists can aid the development of consistent benchmarks that allow evaluation of both stand-alone ML and hybrids in terms of geophysical consistency¹²⁰. However, the help of the AI community is needed to resolve other recently highlighted ML pitfalls. For example, identifying and avoiding shortcut learning¹²¹ in hybrid models, developing ESM concepts of adversarial examples and deep learning artifacts¹²², and developing additive feature attribution¹²³ tools appropriate for physical applications such as within XAI¹¹⁰. Only through combined efforts and the continuous development of both ESMs and AI can NESYM emerge.

Concluding remarks

Our Perspective should not only be seen as the outline of a promising scientific pathway to achieving a better understanding of the Earth’s present and future state, but also as an answer to the recent call for collaboration from the AI community¹²⁴. It can be seen from current applications of AI to Earth system and climate sciences that further exploration of the full potential and, equally, the limits of AI in this field are important. Yet, this line of research is a high-risk venture with many potential pitfalls and dead ends. At this point, there is no guarantee that AI will be the key to overcoming the grand challenges of Earth and climate sciences, some of which were

described at the beginning of this Perspective. In its current stage, it also seems unlikely that AI alone can solve the climate prediction problem. In the coming years, AI will necessarily need to rely on clear, physically meaningful research hypotheses, the geophysical determinism of process-based modelling and careful human evaluation against domain-specific knowledge. Along such lines, we believe that lasting progress beyond the current hype in applying AI to Earth system science will be possible. However, once we find solutions to the foreseeable limitations described above and can build interpretable and geophysically consistent AI tools, this next evolutionary step will seem much more likely.

Received: 12 January 2021; Accepted: 28 June 2021;

Published online: 17 August 2021

References

- Prinn, R. G. Development and application of earth system models. *Proc. Natl Acad. Sci. USA* **110**, 3673–3680 (2013).
- Taylor, K. E., Stouffer, R. J. & Meehl, G. A. An overview of CMIP5 and the experiment design. *Bull. Am. Meteorol. Soc.* **93**, 485–498 (2012).
- IPCC *Climate Change 2013: The Physical Science Basis* (eds Stocker, T. F. et al.) (Cambridge Univ. Press, 2013).
- Eyring, V. et al. Overview of the Coupled Model Intercomparison Project Phase 6 (CMIP6) experimental design and organization. *Geosci. Model Dev.* **9**, 1937–1958 (2016).
- Lin, J. W.-B. & Neelin, J. D. Considerations for stochastic convective parameterization. *J. Atmos. Sci.* **59**, 959–975 (2002).
- Klein, R. Scale-dependent models for atmospheric flows. *Annu. Rev. Fluid Mech.* **42**, 249–274 (2010).
- Berner, J. et al. Stochastic parameterization: toward a new view of weather and climate models. *Bull. Am. Meteorol. Soc.* **98**, 565–588 (2017).
- Knutti, R. Should we believe model predictions of future climate change? *Phil. Trans. R. Soc. A* **366**, 4647–4664 (2008).
- Knutti, R., Rugenstein, M. A. & Hegerl, G. C. Beyond equilibrium climate sensitivity. *Nat. Geosci.* **10**, 727–736 (2017).
- Meehl, G. A. et al. Context for interpreting equilibrium climate sensitivity and transient climate response from the CMIP6 Earth system models. *Sci. Adv.* **6**, eaba1981 (2020).
- Zelinka, M. D. et al. Causes of higher climate sensitivity in CMIP6 models. *Geophys. Res. Lett.* **47**, e2019GL085782 (2020).
- Lenton, T. M. et al. Tipping elements in the earth’s climate system. *Proc. Natl Acad. Sci. USA* **105**, 1786–1793 (2008).
- Boers, N., Ghil, M. & Rousseau, D.-D. Ocean circulation, ice shelf, and sea ice interactions explain Dansgaard-Oeschger cycles. *Proc. Natl Acad. Sci. USA* **115**, E11005–E11014 (2018).
- Valdes, P. Built for stability. *Nat. Geosci.* **4**, 414–416 (2011).
- Drijfhout, S. et al. Catalogue of abrupt shifts in Intergovernmental Panel on Climate Change climate models. *Proc. Natl Acad. Sci. USA* **112**, E5777–E5786 (2015).
- IPCC *Special Report on Global Warming of 1.5°C* (eds Masson-Delmotte, V. et al.) (WMO, 2018); <https://www.ipcc.ch/sr15>
- IPCC *Special Report on Climate Change and Land* (eds Shukla, P. et al.) (IPCC, 2019); <https://www.ipcc.ch/srcl/>
- IPCC *Special Report on the Ocean and Cryosphere in a Changing Climate* (eds Pörtner, H. et al.) (IPCC, 2019); <https://www.ipcc.ch/srocc/>
- Otto, F. E. et al. Attribution of extreme weather events in Africa: a preliminary exploration of the science and policy implications. *Climatic Change* **132**, 531–543 (2015).
- Balsamo, G. et al. Satellite and in situ observations for advancing global earth surface modelling: a review. *Remote Sens.* **10**, 2038 (2018).
- Hersbach, H. et al. The ERA5 global reanalysis. *Q. J. R. Meteorol. Soc.* **146**, 1999–2049 (2020).
- Evensen, G. *Data Assimilation: The Ensemble Kalman Filter* (Springer, 2009).
- Houtekamer, P. L. & Zhang, F. Review of the ensemble Kalman filter for atmospheric data assimilation. *Mon. Weather Rev.* **144**, 4489–4532 (2016).
- van Leeuwen, P. J. Nonlinear data assimilation in geosciences: an extremely efficient particle filter. *Q. J. R. Meteorol. Soc.* **136**, 1991–1999 (2010).
- van Leeuwen, P. J., Künsch, H. R., Nerger, L., Pothast, R. & Reich, S. Particle filters for high-dimensional geoscience applications: a review. *Q. J. R. Meteorol. Soc.* **145**, 2335–2365 (2019).
- Vetra-Carvalho, S. et al. State-of-the-art stochastic data assimilation methods for high-dimensional non-Gaussian problems. *Tellus A* **70**, 1–43 (2018).
- Penny, S. G. et al. Strongly coupled data assimilation in multiscale media: experiments using a quasi-geostrophic coupled model. *J. Adv. Model. Earth Syst.* **11**, 1803–1829 (2019).

28. Browne, P. A., de Rosnay, P., Zuo, H., Bennett, A. & Dawson, A. Weakly coupled ocean-atmosphere data assimilation in the ECMWF NWP system. *Remote Sens.* **11**, 234 (2019).
29. Voulodimos, A., Doulamis, N., Doulamis, A. & Protopapadakis, E. Deep learning for computer vision: a brief review. *Comput. Intell. Neurosci.* **2018**, 7068349 (2018).
30. Brown, T. B. et al. Language models are few-shot learners. Preprint at <https://arxiv.org/abs/2005.14165> (2020).
31. Loh, E. Medicine and the rise of the robots: a qualitative review of recent advances of artificial intelligence in health. *BMJ Lead.* **2**, 59–63 (2018).
32. Girasa, R. in *Artificial Intelligence as a Disruptive Technology* 3–21 (Springer, 2020).
33. Bauer, P. et al. The digital revolution of Earth-system science. *Nat. Comput. Sci.* **1**, 104–113 (2021).
34. Lary, D. J., Alavi, A. H., Gandomi, A. H. & Walker, A. L. Machine learning in geosciences and remote sensing. *Geosci. Front.* **7**, 3–10 (2016).
35. Salcedo-Sanz, S. et al. Machine learning information fusion in Earth observation: a comprehensive review of methods, applications and data sources. *Inf. Fusion* **63**, 256–272 (2020).
36. Dawson, M., Olvera, J., Fung, A. & Manry, M. Inversion of surface parameters using fast learning neural networks. In *Proc. IGARSS '92 International Geoscience and Remote Sensing Symposium Vol. 2*, 910–912 (IEEE, 1992); <http://ieeexplore.ieee.org/document/578294>
37. Miller, D. M., Kaminsky, E. J. & Rana, S. Neural network classification of remote-sensing data. *Comput. Geosci.* **21**, 377–386 (1995).
38. Serpico, S. B., Bruzzone, L. & Roli, F. An experimental comparison of neural and statistical non-parametric algorithms for supervised classification of remote-sensing images. *Pattern Recogn. Lett.* **17**, 1331–1341 (1996).
39. Hsieh, W. W. & Tang, B. Applying neural network models to prediction and data analysis in meteorology and oceanography. *Bull. Am. Meteorol. Soc.* **79**, 1855–1870 (1998).
40. Knutti, R., Stocker, T. F., Joos, F. & Plattner, G. K. Probabilistic climate change projections using neural networks. *Clim. Dynam.* **21**, 257–272 (2003).
41. Arcomano, T. et al. A machine learning-based global atmospheric forecast model. *Geophys. Res. Lett.* **47**, e2020GL087776 (2020).
42. Weyn, J. A., Durran, D. R. & Caruana, R. Can machines learn to predict weather? Using deep learning to predict gridded 500-hPa geopotential height from historical weather data. *J. Adv. Model. Earth Syst.* **11**, 2680–2693 (2019).
43. Weyn, J. A., Durran, D. R. & Caruana, R. Improving data-driven global weather prediction using deep convolutional neural networks on a cubed sphere. *J. Adv. Model. Earth Syst.* **12**, e2020MS002109 (2020).
44. Chantry, M., Hatfield, S., Duben, P., Polichtchouk, I. & Palmer, T. Machine learning emulation of gravity wave drag in numerical weather forecasting. Preprint at <https://arxiv.org/abs/2101.08195> (2021).
45. Gettelman, A. et al. Machine learning the warm rain process. *J. Adv. Model. Earth Syst.* **13**, e2020MS002268 (2021).
46. Rasp, S. & Thuerey, N. Data-driven medium-range weather prediction with a Resnet pretrained on climate simulations: a new model for WeatherBench. *J. Adv. Model. Earth Syst.* **13**, e2020MS002405 (2021).
47. Palmer, T. A vision for numerical weather prediction in 2030. Preprint at <https://arxiv.org/abs/2007.04830> (2020).
48. Neumann, P. et al. Assessing the scales in numerical weather and climate predictions: will exascale be the rescue? *Phil. Trans. R. Soc. A* **377**, 20180148 (2019).
49. Kurth, T. et al. Exascale deep learning for climate analytics. In *SC18: International Conference for High Performance Computing, Networking, Storage and Analysis* 649–660 (IEEE, 2018).
50. Boers, N. et al. Complex networks reveal global pattern of extreme-rainfall teleconnections. *Nature* **566**, 373–377 (2019).
51. Ham, Y.-g., Kim, J.-h. & Luo, J.-j. Deep learning for multi-year ENSO forecasts. *Nature* **573**, 568–572 (2019).
52. Yan, J., Mu, L., Wang, L., Ranjan, R. & Zomaya, A. Y. Temporal convolutional networks for the advance prediction of ENSO. *Sci. Rep.* **10**, 8055 (2020).
53. Kadow, C., Hall, D. M. & Ulbrich, U. Artificial intelligence reconstructs missing climate information. *Nat. Geosci.* **13**, 408–413 (2020).
54. Barnes, E. A., Hurrell, J. W., Ebert-Uphoff, I., Anderson, C. & Anderson, D. Viewing forced climate patterns through an AI lens. *Geophys. Res. Lett.* **46**, 13389–13398 (2019).
55. Barnes, E. A. et al. Indicator patterns of forced change learned by an artificial neural network. *J. Adv. Model. Earth Syst.* **12**, e2020MS002195 (2020).
56. Chattopadhyay, A., Hassanzadeh, P. & Pasha, S. Predicting clustered weather patterns: a test case for applications of convolutional neural networks to spatio-temporal climate data. *Sci. Rep.* **10**, 1317 (2020).
57. Ramachandran, P., Zoph, B. & Le, Q. V. Searching for activation functions. Preprint at <https://arxiv.org/abs/1710.05941> (2017).
58. Lu, Z., Hunt, B. R. & Ott, E. Attractor reconstruction by machine learning. *Chaos* **28**, 061104 (2018).
59. Rumelhart, D. E., Hinton, G. E. & Williams, R. J. Learning representations by back-propagating errors. *Nature* **323**, 533–536 (1986).
60. Reichstein, M. et al. Deep learning and process understanding for data-driven earth system science. *Nature* **566**, 195–204 (2019).
61. Huntingford, C. et al. Machine learning and artificial intelligence to aid climate change research and preparedness. *Environ. Res. Lett.* **14**, 124007 (2019).
62. Irrgang, C., Saynisch, J. & Thomas, M. Estimating global ocean heat content from tidal magnetic satellite observations. *Sci. Rep.* **9**, 7893 (2019).
63. Irrgang, C., Saynisch-Wagner, J., Dill, R., Boergens, E. & Thomas, M. Self-validating deep learning for recovering terrestrial water storage from gravity and altimetry measurements. *Geophys. Res. Lett.* **47**, e2020GL089258 (2020).
64. Jung, M. et al. Scaling carbon fluxes from eddy covariance sites to globe: synthesis and evaluation of the fluxcom approach. *Biogeosciences* **17**, 1343–1365 (2020).
65. Tramontana, G. et al. Partitioning net carbon dioxide fluxes into photosynthesis and respiration using neural networks. *Glob. Change Biol.* **26**, 5235–5253 (2020).
66. Bolton, T. & Zanna, L. Applications of deep learning to ocean data inference and subgrid parameterization. *J. Adv. Model. Earth Syst.* **11**, 376–399 (2019).
67. Rasp, S., Pritchard, M. S. & Gentile, P. Deep learning to represent subgrid processes in climate models. *Proc. Natl Acad. Sci.* **115**, 9684–9689 (2018).
68. O’Gorman, P. A. & Dwyer, J. G. Using machine learning to parameterize moist convection: potential for modeling of climate, climate change, and extreme events. *J. Adv. Model. Earth Syst.* **10**, 2548–2563 (2018).
69. Gagne, D. J., Christensen, H. M., Subramanian, A. C. & Monahan, A. H. Machine learning for stochastic parameterization: generative adversarial networks in the Lorenz ’96 model. *J. Adv. Model. Earth Syst.* **12**, e2019MS001896 (2020).
70. Han, Y., Zhang, G. J., Huang, X. & Wang, Y. A moist physics parameterization based on deep learning. *J. Adv. Model. Earth Syst.* **12**, e2020MS002076 (2020).
71. Beucler, T., Pritchard, M., Gentile, P. & Rasp, S. Towards physically-consistent, data-driven models of convection. Preprint at <https://arxiv.org/abs/2002.08525> (2020).
72. Yuval, J. & O’Gorman, P. A. Stable machine-learning parameterization of subgrid processes for climate modeling at a range of resolutions. *Nat. Commun.* **11**, 3295 (2020).
73. Brenowitz, N. D. & Bretherton, C. S. Prognostic validation of a neural network unified physics parameterization. *Geophys. Res. Lett.* **45**, 6289–6298 (2018).
74. Watt-Meyer, O. et al. Correcting weather and climate models by machine learning nudged historical simulations. Preprint at ESSOAr <https://doi.org/10.1002/essoar.10505959.1> (2021).
75. Pathak, J. et al. Hybrid forecasting of chaotic processes: using machine learning in conjunction with a knowledge-based model. *Chaos* **28**, 041101 (2018).
76. Krasnopolsky, V. M. & Fox-Rabinovitz, M. S. Complex hybrid models combining deterministic and machine learning components for numerical climate modeling and weather prediction. *Neural Netw.* **19**, 122–134 (2006).
77. Brenowitz, N. D. et al. Machine learning climate model dynamics: offline versus online performance. Preprint at <https://arxiv.org/abs/2011.03081> (2020).
78. Brenowitz, N. D., Beucler, T., Pritchard, M. & Bretherton, C. S. Interpreting and stabilizing machine-learning parametrizations of convection. *J. Atmos. Sci.* **77**, 4357–4375 (2020).
79. Seifert, A. & Rasp, S. Potential and limitations of machine learning for modeling warm-rain cloud microphysical processes. *J. Adv. Model. Earth Syst.* **12**, e2020MS002301 (2020).
80. Beucler, T., Rasp, S., Pritchard, M. & Gentile, P. Achieving conservation of energy in neural network emulators for climate modeling. Preprint at <https://arxiv.org/abs/1906.06622> (2019).
81. Schneider, T., Lan, S., Stuart, A. & Teixeira, J. Earth system modeling 2.0: a blueprint for models that learn from observations and targeted high-resolution simulations. *Geophys. Res. Lett.* **44**, 12396–12417 (2017).
82. Cintra, R. S. & Velho, H. F. C. Data assimilation by artificial neural networks for an atmospheric general circulation model: conventional observation. *Bull. Am. Meteorological Soc.* **77**, 437–471 (2014).
83. Wahle, K., Staneva, J. & Guenther, H. Data assimilation of ocean wind waves using neural networks. a case study for the german bight. *Ocean Model.* **96**, 117–125 (2015).

84. Irrgang, C., Saynisch-Wagner, J. & Thomas, M. Machine learning-based prediction of spatiotemporal uncertainties in global wind velocity reanalyses. *J. Adv. Model. Earth Syst.* **12**, e2019MS001876 (2020).
85. Brajard, J., Carrassi, A., Bocquet, M. & Bertino, L. Combining data assimilation and machine learning to emulate a dynamical model from sparse and noisy observations: a case study with the Lorenz 96 model. *J. Comput. Sci.* **44**, 101171 (2020).
86. Ruckstuhl, Y., Janjić, T. & Rasp, S. Training a convolutional neural network to conserve mass in data assimilation. *Nonlin. Processes Geophys.* **28**, 111–119 (2020).
87. Geer, A. J. Learning Earth system models from observations: machine learning or data assimilation? *Phil. Trans. R. Soc. A* **379**, 20200089 (2021).
88. Runge, J. et al. Inferring causation from time series in Earth system sciences. *Nat. Commun.* **10**, 2553 (2019).
89. Boers, N. et al. Prediction of extreme floods in the eastern central andes based on a complex networks approach. *Nat. Commun.* **5**, 5199 (2014).
90. Qi, D. & Majda, A. J. Using machine learning to predict extreme events in complex systems. *Proc. Natl Acad. Sci. USA* **117**, 52–59 (2020).
91. Sonnewald, M., Dutkiewicz, S., Hill, C. & Forget, G. Elucidating ecological complexity: unsupervised learning determines global marine eco-provinces. *Sci. Adv.* **6**, 1–12 (2020).
92. Leinonen, J., Guillaume, A. & Yuan, T. Reconstruction of cloud vertical structure with a generative adversarial network. *Geophys. Res. Lett.* **46**, 7035–7044 (2019).
93. Stengel, K., Glaws, A., Hettinger, D. & King, R. N. Adversarial super-resolution of climatological wind and solar data. *Proc. Natl Acad. Sci. USA* **117**, 16805–16815 (2020).
94. Huber, M. & Knutti, R. Anthropogenic and natural warming inferred from changes in Earth's energy balance. *Nat. Geosci.* **5**, 31–36 (2012).
95. Zanna, L. & Bolton, T. Data-driven equation discovery of ocean mesoscale closures. *Geophys. Res. Lett.* **47**, e2020GL088376 (2020).
96. Lagaris, I. E., Likas, A. & Fotiadis, D. I. Artificial neural networks for solving ordinary and partial differential equations. *IEEE Trans. Neural Netw.* **9**, 987–1000 (1998).
97. Raissi, M., Perdikaris, P. & Karniadakis, G. Physics-informed neural networks: a deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J. Comput. Phys.* **378**, 686–707 (2019).
98. Ramadhan, A. et al. Capturing missing physics in climate model parameterizations using neural differential equations. Preprint at <http://arxiv.org/abs/2010.12559> (2020).
99. Goodfellow, I. J. et al. Generative adversarial networks. Preprint at <https://arxiv.org/abs/1406.2661> (2014).
100. Hurrell, J. W. et al. The Community Earth System Model: a framework for collaborative research. *Bull. Am. Meteorol. Soc.* **94**, 1339–1360 (2013).
101. Rudin, C. Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. *Nat. Mach. Intell.* **1**, 206–215 (2019).
102. Balaji, V. Climbing down Charney's ladder: machine learning and the post-Dennard era of computational climate science. *Phil. Trans. R. Soc. A* **379**, 20200085 (2021).
103. Sonnewald, M. et al. Bridging observation, theory and numerical simulation of the ocean using machine learning. Preprint at <https://arxiv.org/abs/2104.12506> (2021).
104. *Ethics Guidelines for Trustworthy AI* (European Commission, 2019); <https://ec.europa.eu/digital-single-market/en/news/ethics-guidelines-trustworthy-ai>
105. *The Biden Administration Launches AI.gov Aimed at Broadening Access to Federal Artificial Intelligence Innovation Efforts, Encouraging Innovators of Tomorrow* (White House, 2021); <https://www.whitehouse.gov/ostp/news-updates/2021/05/05/the-biden-administration-launches-ai-gov-aimed-at-broadening-access-to-federal-artificial-intelligence-innovation-efforts-encouraging-innovators-of-tomorrow/>
106. Toms, B. A., Barnes, E. A. & Ebert-Uphoff, I. Physically interpretable neural networks for the geosciences: applications to Earth system variability. *J. Adv. Model. Earth Syst.* **12**, e2019MS002002 (2020).
107. Kaiser, B. E., Saenz, J. A., Sonnewald, M. & Livescu, D. Objective discovery of dominant dynamical processes with intelligible machine learning. Preprint at <https://arxiv.org/abs/2106.12963> (2021).
108. McGovern, A. et al. Making the black box more transparent: understanding the physical implications of machine learning. *Bull. Am. Meteorological Soc.* **100**, 2175–2199 (2019).
109. Ebert-Uphoff, I. & Hilburn, K. Evaluation, tuning and interpretation of neural networks for working with images in meteorological applications. *B. Am. Meteorol. Soc.* **101**, E2149–E2170 (2020).
110. Sonnewald, M. & Iguensat, R. Revealing the impact of global heating on North Atlantic circulation using transparent machine learning. Preprint at ESSOAr <https://doi.org/10.1002/essoar.10506146.1> (2021).
111. Beucler, T., Ebert-Uphoff, I., Rasp, S., Pritchard, M. & Gentine, P. Machine learning for clouds and climate (invited chapter for the AGU geophysical monograph series 'clouds and climate'). Preprint at ESSOAr <https://doi.org/10.1002/essoar.10506925.1> (2021).
112. Olden, J. D., Joy, M. K. & Death, R. G. An accurate comparison of methods for quantifying variable importance in artificial neural networks using simulated data. *Ecol. Model.* **178**, 389–397 (2004).
113. Bach, S. et al. On pixel-wise explanations for non-linear classifier decisions by layer-wise relevance propagation. *PLoS ONE* **10**, e0130140 (2015).
114. Barnes, E. A., Mayer, K., Toms, B., Martin, Z. & Gordon, E. Identifying opportunities for skillful weather prediction with interpretable neural networks. Preprint at <https://arxiv.org/abs/2012.07830> (2020).
115. Sonnewald, M., Wunsch, C. & Heimbach, P. Unsupervised learning reveals geography of global ocean dynamical regions. *Earth Space Sci.* **6**, 784–794 (2019).
116. Callahan, J. L., Koch, J. V., Brunton, B. W., Kutz, J. N. & Brunton, S. L. Learning dominant physical processes with data-driven balance models. *Nat. Commun.* **12**, 1016 (2021).
117. Runge, J., Nowack, P., Kretschmer, M., Flaxman, S. & Sejdinovic, D. Detecting and quantifying causal associations in large nonlinear time series datasets. *Sci. Adv.* **5**, eaau4996 (2019).
118. Eyring, V. et al. Taking climate model evaluation to the next level. *Nat. Clim. Change* **9**, 102–110 (2019).
119. Schlund, M. et al. Constraining uncertainty in projected gross primary production with machine learning. *J. Geophys. Res. Biogeosci.* **125**, e2019JG005619 (2020).
120. Rasp, S. et al. WeatherBench: a benchmark dataset for data-driven weather forecasting. *J. Adv. Model. Earth Syst.* **12**, e2020MS002203 (2020).
121. Geirhos, R. et al. Shortcut learning in deep neural networks. *Nat. Mach. Intell.* **2**, 665–673 (2020).
122. Buckner, C. Understanding adversarial examples requires a theory of artefacts for deep learning. *Nat. Mach. Intell.* **2**, 731–736 (2020).
123. Alvarez-Melis, D. & Jaakkola, T. S. On the robustness of interpretability methods. Preprint at <https://arxiv.org/abs/1806.08049> (2018).
124. Rolnick, D. et al. Tackling climate change with machine learning. Preprint at <http://arxiv.org/abs/1906.05433> (2019).

Acknowledgements

This study was funded by the Helmholtz Association and by the Initiative and Networking Fund of the Helmholtz Association through the project Advanced Earth System Modelling Capacity (ESM). N.B. acknowledges funding by the Volkswagen foundation and the European Union's Horizon 2020 research and innovation program under grant agreement number 820970 (TiPES, contribution #121). E.A.B. was supported, in part, by the US National Science Foundation under grant number AGS-1749261. M.S. acknowledges funding from the Cooperative Institute for Modeling the Earth System, Princeton University, under award number NA18OAR4320123 and from the National Oceanic and Atmospheric Administration, US Department of Commerce. The statements, findings, conclusions, and recommendations are those of the authors and do not necessarily reflect the views of Princeton University, the National Oceanic and Atmospheric Administration or the US Department of Commerce.

Author contributions

C.I. conceived the study and organized the collaboration. All authors contributed to writing and revising all sections of this manuscript. In particular, N.B. and C.I. drafted the ESM overview, J.S.-W. and J.S. drafted the ESO and data assimilation overview, C.I. and C.K. drafted the 'From ML-based data exploration towards learning physics' section, C.I. and J.S.-W. and N.B. drafted the 'Fusion of process-based models and AI' section and M.S. and E.A.B. and C.I. drafted the 'Peering into the black box' section.

Competing interests

The authors declare no competing interests.

Additional information

Correspondence should be addressed to C.I.

Peer review information *Nature Machine Intelligence* thanks the anonymous reviewers for their contribution to the peer review of this work.

Reprints and permissions information is available at www.nature.com/reprints.

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

© Springer Nature Limited 2021