

UNIVERSITY OF BREMEN
INSTITUTE OF ENVIRONMENTAL PHYSICS (IUP)

Constraining Uncertainties in Multi-Model Projections of the Future Climate with Observations

DISSERTATION

Author:
Manuel SCHLUND

Supervisors:
Prof. Dr. Veronika EYRING
Prof. Dr. Pierre GENTINE

*This thesis is submitted for the degree
Doktor der Naturwissenschaften (Dr. rer. nat.)*

March 2021

Abstract (English version)

TBA.

Abstract (German version)

TBA.

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1. Introduction

1.1. Motivation

- Why is climate change relevant for the society?
 - Cite latest warming reports, also other variables (droughts, extreme events, etc.)
 - basic physics of greenhouse gases (vibration modes, etc.)
 - definition of radiative forcing
 - well-mixed greenhouse gases (water vapor, CO₂, CH₄) + sources
 - long-lived vs. short-lived GHGs?
 - aerosols + cooling effect
 - natural vs. anthropogenic effects (D & A) -> clear evidence that climate change over 21st century is caused by human influence (<https://globalwarmingindex.org/>, Haustein et al., 2017)

1.2. Structure of the Thesis

Parts of this thesis are published in multiple peer-reviewed publications (two first-author studies and six co-author studies). If applicable, this is clearly stated at the beginning of each chapter. Chapter 2 introduces the scientific background for this thesis. This includes relevant literature that is used as a baseline for this thesis. Chapter 3 gives an overview over the contributions made to the Earth System Model Evaluation Tool (ESMValTool), an open-source software for the analysis of Earth System Models (ESMs). These contributions helped improving the routine evaluation of ESMs which is useful for the whole scientific community and lead to co-authorship in four peer-reviewed studies (Eyring et al., 2020; Lauer et al., 2020; Righi et al., 2020; Weigel et al., 2020). Chapter 4 covers the assessment of policy-relevant climate metrics like the Effective Climate Sensitivity (ECS) and the Transient Climate Response (TCR) in the latest generation of ESMs. This work is already published in two scientific publications (Bock et al., 2020; Meehl et al., 2020). Since the ECS and TCR are considerably higher in this

new climate model generation, chapter 5 describes the assessment of emergent constraints (a technique to reduce uncertainties in multi-model climate projections, see section 2.4.1) on the ECS for these ESMs. The contents of this chapter are published in *Earth System Dynamics* (Schlund, Lauer, et al., 2020). Chapter 6 focuses on a new method to reduce uncertainties in multi-model projections of the future climate based on Machine Learning (ML). As an example, the method is applied to the photosynthesis rate at the end of the 21st century, which is already published in the *Journal of Geophysical Research: Biogeosciences* (Schlund, Eyring, et al., 2020). Finally, chapter 7 provides a summary of the results of this thesis and gives an outlook of possible future works.

2. Scientific Background

This chapter introduces the scientific background of this thesis. First, basic concepts of climate model simulations and associated uncertainties are introduced. Next, the fundamental biogeochemical processes of the global carbon cycle and important metrics describing climate change are presented. Finally, state-of-the-art techniques used to reduce uncertainties in projections of the future climate are shown. These methods form the basis for the new techniques developed in this thesis.

2.1. Earth System Models: Simulations and Analysis

2.1.1. Numerical Climate Modeling

In contrast to other fields of science, researching the future evolution of the Earth's climate cannot be purely done by performing experiments in a laboratory. Due to the immense complexity of the Earth system (including physical, biological and chemical processes on various temporal and spatial scales and their mutual interactions), we do not have access to a tiny replica of the Earth that we can analyze when exposed to different external conditions (Flato, 2011). While observing the current state of the Earth System is (relatively) straightforward, gaining evidence about the future evolution of the climate by only considering present-day observations is rather difficult.

A possible way out is given by numerical climate models, which offer the possibility to simulate the Earth's climate on a computer. The first numerical climate models came up in the 1960s and were based on weather prediction models (Flato, 2011). Early models from the 1970s simulated only the physical components of the climate system: atmosphere, land surface, ocean and sea ice (see figure 2.1). The basis of these so-called Atmosphere-Ocean General Circulation Models (AOGCMs) (Flato et al., 2013) is the numerical solving of the differential equations describing the exchange of energy and matter between these physical components.

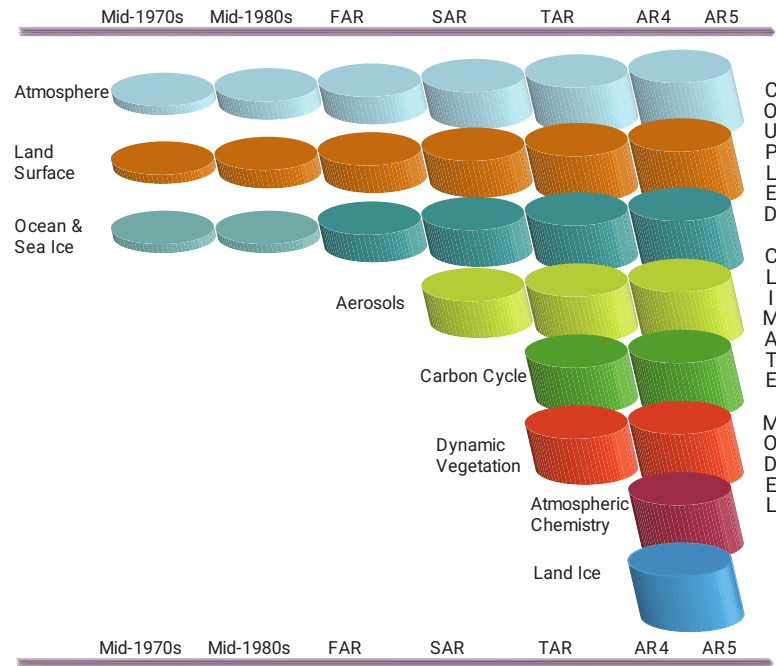


Figure 2.1.: Historical evolution of coupled climate models over the last 45 years. In early days, these models were so-called Atmosphere-Ocean General Circulation Models (AOGCMs) and only included three components: the atmosphere, the land surface and the ocean. Over the time, the individual components grew in complexity and included a wider range of processes (illustrated by the growing cylinders). Eventually, more and more components (aerosols, carbon cycle, etc.) were added to the coupled system, forming the modern Earth System Models (ESMs). Taken from Cubasch et al. (2013).

Over the course of the years, climate models became more and more complex by including a wider range of processes within the components, but also by introducing new components to the coupled system. Examples of these are aerosols, the carbon cycle, a dynamic vegetation, atmospheric chemistry and land ice (see figure 2.1). AOGCMs coupled to these additional components are called Earth System Models (ESMs), which are the current state-of-the-art models that allow the most sophisticated simulations of the Earth's climate. In contrast to AOGCMs, ESMs enable the simulation of biological and chemical processes in addition to the dynamics of the physical components of the Earth system. Especially in the context of anthropogenic climate change, these additional processes are of uttermost importance for realistic climate model simulations, since the anthropogenic interference with the Earth system directly influences the various biogeochemical cycles of the Earth. For example, the emission of the most prominent Greenhouse Gas (GHG), carbon dioxide (CO_2), immediately impacts the global carbon cycle by inserting additional carbon into the system

(for details see section 2.3). Further examples include land use changes like the deforestation of tropical rainforests, which also directly influences several biogeochemical cycles (e.g. carbon cycle, nitrogen cycle, phosphorus cycle, etc.) by altering respective sinks and sources.

Due to the complex interactions between the different components of the Earth system, these changes in the biogeochemical processes also affect the physical properties of the climate system. For example, due to the global carbon cycle, only about 50 % of the emitted CO₂ by humankind remains in the atmosphere (Friedlingstein et al., 2019). The residual part is absorbed by the two other main carbon sinks of the planet, the terrestrial biosphere and the ocean. Since only atmospheric CO₂ can act as GHG by introducing an additional radiative forcing to the Earth System leading to increasing surface temperatures, this uptake of CO₂ by the carbon cycle slows down global warming.

2.1.2. CMIP

Due to the complex nature of the Earth system itself, numerical models of it consist of hundreds of thousands of lines of computer code. Thus, a standardization to a certain degree is crucial for the various research groups developing ESMs all around the world in order to obtain comparable output and to facilitate model analysis. For this reason, the Working Group on Coupled Modelling (WGCM) of the World Climate Research Programme (WCRP) initiated the Coupled Model Intercomparison Project (CMIP) in 1995, with the objective to “better understand past, present and future climate changes arising from natural, unforced variability or in response to changes in radiative forcing in a multi-model context” (WCRP, 2020). One major element of CMIP is to establish common standards, coordination, infrastructure and documentation in order to facilitate the distribution of climate model output (Eyring et al., 2016).

A further main aspect is to provide a set of standardized experiments for global climate model simulations. To participate in the latest phase of CMIP, CMIP6, climate models need to run a *historical* simulation of the period 1850–2014 and the so-called Diagnostic, Evaluation, and Characterisation of Klima (DECK) experiments, which include a pre-industrial control run (*piControl*), a historical Atmospheric Model Intercomparison Project (MIP) simulation (*amip*), a simulation forced with an abrupt quadrupling of CO₂ (*abrupt-4xCO2*) and a simulation forced with a 1 % per year increase of the atmospheric CO₂ concentration (*1pctCO2*) (Eyring et al., 2016). This is shown in the center of figure 2.2, which illustrates the experimental design of CMIP6.

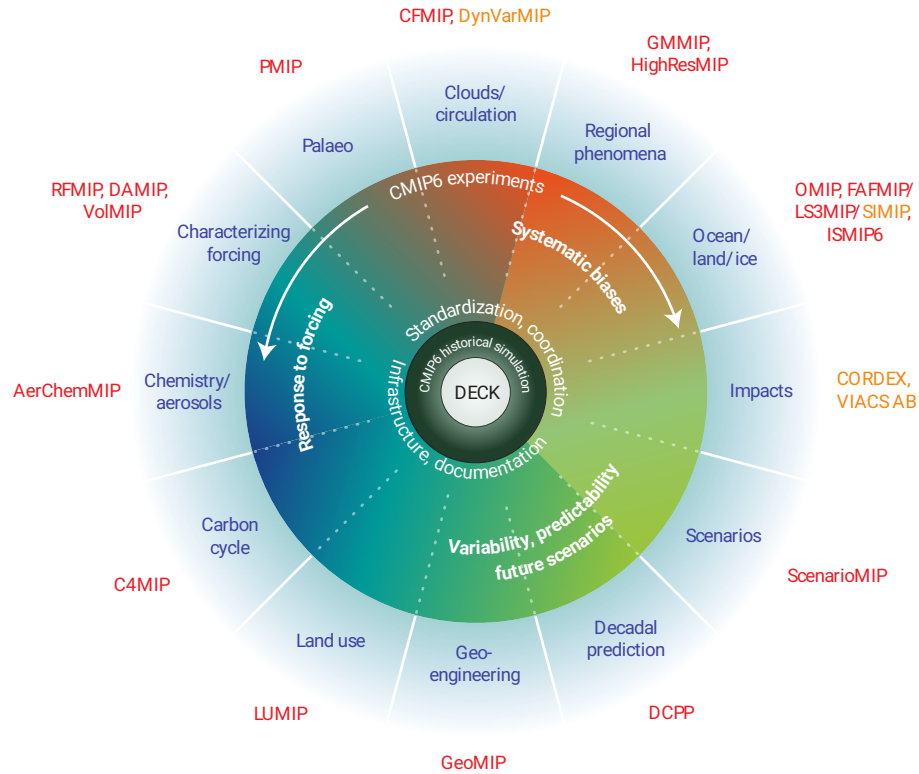


Figure 2.2.: Schematic of the experiment design of Phase 6 of the Coupled Model Intercomparison Project (CMIP6). The center of the circle illustrates the four DECK (Diagnostic, Evaluation, and Characterisation of Klima) experiments and the CMIP6 historical simulation. The circular sectors show additional science themes that can be explored through the 21 CMIP6-Endorsed Model Intercomparison Projects (MIPs). Taken from Simpkins (2017).

To increase diversity and answer more scientific questions, CMIP6 models can participate in the so-called CMIP6-Endorsed MIPs, of which CMIP6 offers 21 (see circular sectors in figure 2.2). Some MIPs offer additional experiments to explore specific aspects of the Earth system, like the Coupled Climate-Carbon Cycle Model Intercomparison Project (C4MIP) which focuses on the carbon cycle (Jones et al., 2016) or the Aerosol Chemistry Model Intercomparison Project (AerChemMIP) which focuses on aerosol chemistry (W. J. Collins et al., 2017). Other MIPs allow the assessment of future climate change. An example is the Scenario Model Intercomparison Project (ScenarioMIP), which provides common experiments that simulate different possible futures (O'Neill et al., 2016). These experiments are based on the so-called Shared Socioeconomic Pathways (SSPs), a set of alternative pathways of future societal development (O'Neill et al., 2017; O'Neill et al., 2013). For each experiment, a set of emissions and land use changes is calculated from the SSPs (Riahi et al., 2017) which

are then used to force the global climate models. For ScenarioMIP, five different SSPs are considered, ranging from SSP1 (sustainability) to SSP5 (fossil-fuel development). Each SSP is combined with a climate outcome (measured as radiative forcing in the year 2100) based on a particular forcing pathway that Integrated Assessment Models (IAMs) have shown to be feasible. For example, SSP5-8.5 represents a scenario based on a fossil-fuel development with a radiative forcing of 8.5 Wm^{-2} in 2100 while SSP1-2.6 represents a sustainable future with a radiative forcing of 2.6 Wm^{-2} in the year 2100. The two scenarios in the main category of ScenarioMIP, the *Tier 1* experiments, are the SSP2-4.5 and SSP3-7.0 scenarios. In contrast to the ScenarioMIP experiments, the corresponding CMIP5 counterparts (Taylor et al., 2012), the so-called Representative Concentration Pathways (RCPs), only used the radiative forcing in 2100 as only dimension to describe the possible futures (e.g. RCP8.5, RCP4.5, RCP2.6, etc.).

In this thesis, climate model data from the two most recent CMIP generations is used, CMIP5 and CMIP6. More detailed information about the specific variables and experiments analyzed is given in the corresponding chapters.

2.1.3. Sources of Uncertainties in Climate Model Projections

Simulations from climate model ensembles of CMIP allow us to assess the impact of future climate change in a consistent and transparent way. Especially the ScenarioMIP experiments can give valuable insights into the upcoming development of the Earth system by providing *projections* of the future climate. In contrast to climate predictions, climate projections run over multiple decades and depend upon the future scenario considered, which are based on assumptions that may or may not turn out to be correct. On the contrary, climate predictions are attempts to predict the actual evolution of the climate on much shorter time scales from seasons to years. Similar to any other scientific experiment, climate model projections suffer from associated uncertainties. There are three major sources of climate model projections we can distinguish: natural variability, climate response uncertainty and emission uncertainty (Hawkins & Sutton, 2009, 2010). Figure 2.3 shows these three sources for the projected global mean surface temperature anomaly over the 21st century.

Natural variability is connected to the chaotic nature of the Earth system that arises from complex interactions between the ocean, atmosphere, land, biosphere and cryosphere (Cubasch et al., 2013). It constitutes a fundamental limit of how precisely we can project the future climate since it is inherent in the Earth system and cannot be eliminated by more knowledge and more advanced

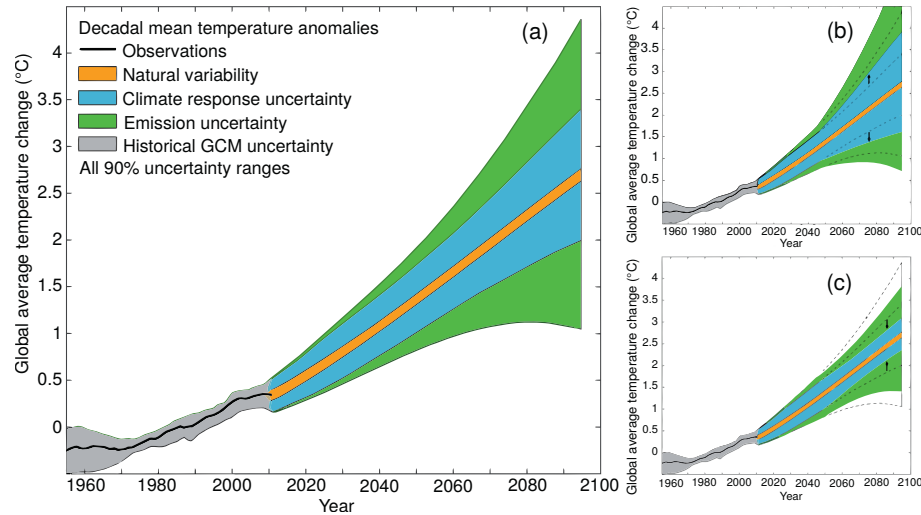


Figure 2.3.: Schematic illustrating the importance of different sources of uncertainties in climate model projections and their evolution in time. (a) Time series of the anomaly of the decadal and global mean surface temperature relative to the period 1961–1980. The black line shows the historical observations with estimates of uncertainty from climate models (gray). The remaining colors show different sources of uncertainty in future climate projections: Natural variability (orange), climate response uncertainty (blue) and emission uncertainty (green) (Hawkins & Sutton, 2009, 2010). Climate response uncertainty can (b) increase in newer generations of climate models when a new process is discovered to be relevant or (c) decrease with additional model improvements and observational constraints. Taken from Cubasch et al. (2013).

climate models. Natural variability is more relevant on regional and local scales than on continental or global scales. Further contributions to natural variability on longer time scales come from phenomena like the El Niño-Southern Oscillation (ENSO) or the North Atlantic Oscillation (NAO) and from externally (and thus explainable) events like volcanic eruptions and variations in the solar activity. Natural variability can be seen as the *noise* in the climate record as opposed to the anthropogenic *signal* (Cubasch et al., 2013). As illustrated by figure 2.3, the uncertainty associated with natural variability is constant over time.

The second source of uncertainty in climate model projections is *emission uncertainty*. This arises from the different possible trajectories in terms of future forcing (GHGs, aerosols, land use changes, etc.) humankind might take. Examples for these are the SSP-based experiments given by ScenarioMIP that include a variety of different scenarios from a sustainable future to a full fossil fuel-based development (see section 2.1.2). A possible approach to quantify emission uncertainty is to assess the climate impact of these different trajectories. Since the emission uncertainty strongly depends on the future development of the human

society, it cannot be reduced by improving climate models. In contrast to natural variability, the emission uncertainty increases over time in climate projections, since estimating forcings for the near future is simpler than for the far future.

Finally, the third source of uncertainty in climate model projections is the *climate response uncertainty*, which comes from our imperfect knowledge of how the climate system will respond to anthropogenic forcings. Due to the complexity of the Earth system, the future climate could develop in many different ways that are all consistent with our current knowledge and models (Cubasch et al., 2013). In the context of climate model ensembles, the climate response uncertainty is often also called *model uncertainty* and reflects the different responses of the different climate models to a given forcing. Even though all climate models are built on the same physical principles, they differ in terms of spatial resolution, processes included and parametrizations of unresolved processes. The latter can be thought of as different approximations that are necessary to represent processes that take place on scales smaller than the common size of grid boxes in modern global climate models (about $1^\circ \times 1^\circ$ horizontally), which is for example the case for cloud processes and vegetation processes.

These differences in the climate models also give rise to different intensities of *climate feedbacks* (or even their presence/absence) in the models. A climate feedback is a mechanism that either amplifies (*positive feedback*) or diminishes (*negative feedback*) the effect of an external forcing. An example of a strong positive feedback is the water vapor feedback, in which the increased surface temperature (caused by anthropogenic forcing) leads to an enhanced evaporation of water which increases the amount of water vapor in the atmosphere. Since water vapor itself is a powerful GHG, this amplifies the effect of the anthropogenic forcing by further increasing the surface temperatures (Cubasch et al., 2013). Further examples and a mathematical framework for the analysis of feedbacks are given in section 2.2.1.

As sciences evolves, representations of already included processes can be improved in climate models. Moreover, new geophysical and biogeochemical processes can be added to them. On the one hand, this can increase the climate response uncertainty when a new process is discovered to be relevant (Cubasch et al., 2013; see figure 2.3b). However, such an increase corresponds to a previously unmeasured uncertainty. An example for this has recently happened in CMIP6: most likely due to changes in the cloud representation of the models the spread in the projected global mean near-surface air temperature (GSAT) caused by a doubling of the atmospheric CO₂ concentration has substantially increased in CMIP6 compared to older CMIP generations (Zelinka et al., 2020).

On the other hand, the climate response uncertainty can decrease with additional model improvements and better understanding of the Earth system (see figure 2.3c). Moreover, it can also be reduced by observational constraints, which is the main topic of this thesis.

2.2. Climate Sensitivity

Climate sensitivity refers to the change in GSAT that results from a change in the radiative forcing. In other words, it describes how sensitive the climate system is to an external forcing. The source of this forcing might either be natural (changes in the solar activity, volcanic eruptions, etc.) or anthropogenic (emissions of GHGs, land use changes, etc.).

2.2.1. Climate Feedbacks

As already described in section 2.1.3, the effects of an external forcing acting on the climate system can additionally be amplified or diminished by climate feedbacks. Thus, feedback processes play a crucial role in the evaluation of climate sensitivity. Figure 2.4 shows an overview of important feedbacks in the Earth system with their corresponding time scales on which they operate.

An example for a positive feedback is the already mentioned *water vapor feedback*. Being the primary GHG in the Earth's atmosphere, water vapor is the largest contributor to the natural greenhouse effect. Since its amount in the atmosphere is mainly controlled by the air temperature and anthropogenic emissions of water vapor are negligible, the influence of water vapor on the climate system is described as a feedback mechanism and not as an external forcing (Myhre et al., 2013). Basis of this feedback is the enhanced evaporation of water with increasing air temperatures. Each degree of warming allows the atmosphere to retain about 7 % more water vapor (Myhre et al., 2013), which closes the positive feedback loop by further increasing air temperatures through the greenhouse effect. With a typical residence time of water vapor in the atmosphere of several days, the water vapor feedback operates on relatively short time scales. As the largest positive feedback in the Earth system (Soden & Held, 2006), the water vapor feedback amplifies any initial forcing (e.g. caused by anthropogenic CO₂ emissions) by a typical factor between two and three, rendering water vapor a fundamental agent of climate change (Myhre et al., 2013). An example for a positive feedback that operates on longer time scales (several years) is the *snow/ice albedo feedback*, in which the surface albedo decreases as

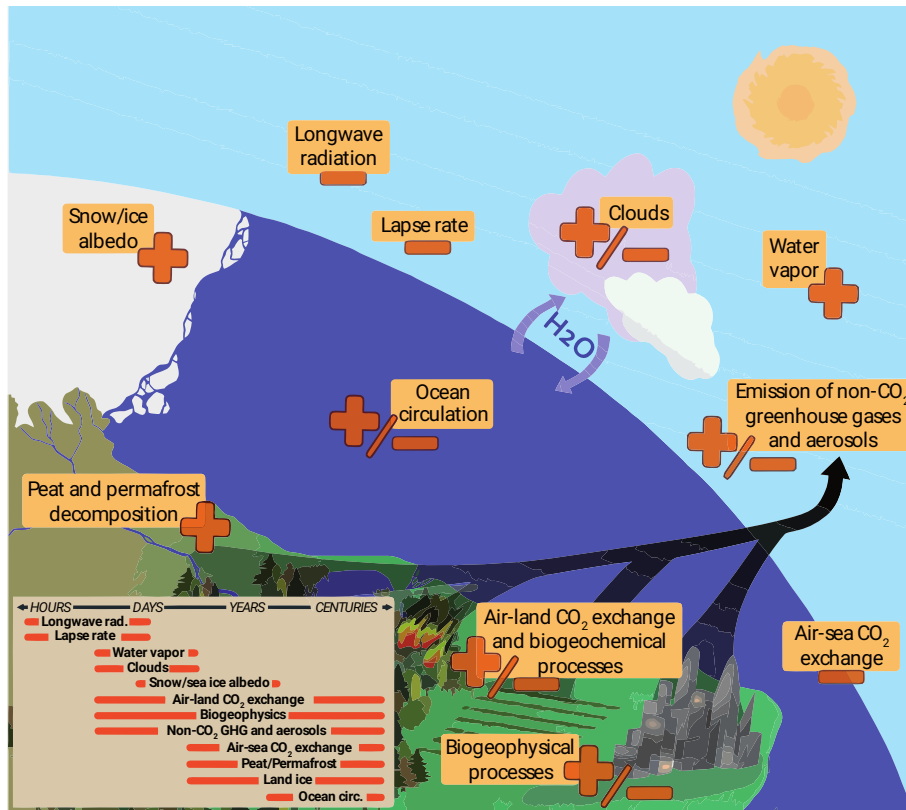


Figure 2.4.: Climate feedbacks and corresponding time scales. “+” refers to positive feedbacks, which amplify the effect of the external forcing (e.g. the water vapor feedback). “-” refers to negative feedbacks, which diminish the effect of the external forcing (e.g. the longwave radiation feedback). “+/-” refers to feedbacks which might be either positive or negative (e.g. the cloud feedback). The smaller box highlights the large differences in time scales for the various feedbacks. Taken from Cubasch et al. (2013).

highly reflective ice and snow surfaces melt with global warming, exposing the darker and more absorbing surfaces below (Cubasch et al., 2013).

In contrast to positive feedbacks, negative feedbacks diminish the effect of an external forcing. An example for this is the *blackbody feedback* (also known as *Planck feedback* or *longwave radiation feedback*), which is the strongest negative feedback in the Earth system (Cubasch et al., 2013). It is based on the thermal electromagnetic radiation that any object with a non-zero temperature emits (the so-called *blackbody radiation*). Since the power of this radiation strongly depends on the temperature of the object, higher surface temperatures of the Earth increase the outgoing longwave radiation flux from the surface which reduces the effect of the external forcing and cools the planet.

For some domains of the Earth system, feedbacks can be positive and/or negative, since a variety of different mechanisms is involved. An example for this

is the cloud feedback. Changes in clouds induced by climate change can cause both longwave (greenhouse warming) and shortwave (reflective cooling) effects, which both need to be considered for the overall cloud feedback (Boucher et al., 2013). Relevant cloud properties that may change as a response to an external forcing and that may alter the Earth's radiative budget are cloud cover, cloud optical thickness, cloud altitude and the geographical distribution of clouds. Examples for robust cloud feedback processes are the rise of high clouds in a warming climate which traps longwave radiation and enhances global warming and the reduction in mid- and low-level cloud cover which diminishes the reflection of incoming solar radiation and also increases the surface warming (Boucher et al., 2013). In global climate model ensembles, the overall cloud feedback shows a large range with positive and negative values, but tends to be slightly positive on average (Dufresne & Bony, 2008; Soden & Held, 2006; Vial et al., 2013; Zelinka et al., 2020). This large uncertainty in the cloud feedback is a major reason for uncertainties in the climate sensitivity of climate models (Boucher et al., 2013; Flato et al., 2013).

Further examples of feedbacks with positive and negative contributions are biogeochemical feedbacks. Negative contributions come from increased CO₂ fluxes into the land and ocean carbon reservoirs due to increased photosynthesis rates and CO₂ dissolution in the sea, respectively, which decrease the atmospheric CO₂ content and diminish global warming. An example for a positive contribution is the decreased solubility of CO₂ in water in a warmer climate, which reduces the atmosphere-ocean CO₂ flux and enhances climate change. More details on this are given in section 2.3.2.

2.2.2. Mathematical Framework for Feedbacks Analysis

The foundation of a basic mathematical framework for climate feedback analysis is a simple energy balance model (Gregory et al., 2009; Roe, 2009). Anthropogenic activities in the Earth system like the emissions of GHGs or aerosols introduce an external forcing to the climate system, which is quantified with a radiative forcing F measured in Wm^{-2} . To restore a stable state, the climate system opposes this forcing with a climate response R , leading to a net energy flux of

$$N = F + R \quad (2.1)$$

into the system. Positive values of N , F and R indicate incoming fluxes; usually $F > 0$ and $R < 0$. On long time scales (multiple years), the net incoming radiative flux at the top of the atmosphere (TOA) and the net heat flux into the

ocean are basically equal definitions of N since nearly all of the Earth's heat capacity resides in the ocean (Gregory et al., 2009). While $N \neq 0$, the climate system evolves; when $N = 0$ a new steady state has been reached.

To quantify the effects of different feedbacks, a reference system with a basic response needs to be defined, which is a crucial aspect of feedback analysis (Roe, 2009). Usually, the idealization of a blackbody Earth without an atmosphere is used for that: In equilibrium, the incoming solar irradiance is balanced with an outgoing thermal irradiance J_0 that solely depends on the global mean surface temperature T_0 following the Stefan–Boltzmann law

$$J_0 = -\sigma T_0^4. \quad (2.2)$$

$\sigma \approx 5.67 \text{ Wm}^{-2}\text{K}^{-4}$ is the Stefan–Boltzmann constant. To answer an external forcing F , the climate system reacts with a response R expressed by a change in the global mean surface temperature ΔT :

$$J_0 + R = -\sigma (T_0 + \Delta T)^4. \quad (2.3)$$

Since the temperature change caused by an anthropogenic forcing is much smaller than the equilibrium temperature $\Delta T \ll T_0 \approx 255 \text{ K}$, a simple first-order Taylor expansion can be used to linearize the blackbody response:

$$-\sigma (T_0 + \Delta T)^4 \approx J_0 - 4\sigma T_0^3 \cdot \Delta T. \quad (2.4)$$

Thus, by comparing equations (2.3) and (2.4) the climate response R can be expressed as

$$R = -4\sigma T_0^3 \cdot \Delta T := \lambda_{\text{BB}} \cdot \Delta T \quad (2.5)$$

with the blackbody feedback parameter $\lambda_{\text{BB}} \approx -3.8 \text{ Wm}^{-2}\text{K}^{-1}$. Results from climate models and analyses of observations confirm this linear relationship between R and ΔT (Gregory et al., 2004). However, the value of this linear constant λ , the *climate feedback parameter*, is found to be considerably larger than the blackbody response ($\lambda \approx -1.0 \text{ Wm}^{-2}\text{K}^{-1}$), indicating that additional processes affect the Earth's radiative balance: the climate feedbacks (Flato et al., 2013; Gregory et al., 2009). Since climate models suggest that the radiative effects of these additional feedbacks are also proportional to ΔT (Gregory & Webb, 2008), equation (2.5) can be adjusted to

$$R = \lambda \cdot \Delta T = (\lambda_{\text{BB}} + \lambda_{\text{WV}} + \lambda_{\text{Albedo}} + \lambda_{\text{Cloud}} + \dots) \cdot \Delta T. \quad (2.6)$$

λ_{WV} refers to the water vapor feedback, λ_{Albedo} to the snow/ice albedo feedback and λ_{Cloud} to the cloud feedback. Thus, the overall climate feedback parameter λ can be written as the sum of the individual feedback parameters λ_i :

$$\lambda = \sum_i \lambda_i. \quad (2.7)$$

Positive values of λ_i indicate positive feedbacks (e.g. the water vapor feedback) and negative values indicate negative feedbacks (e.g. the blackbody feedback). This equation assumes that the individual radiative responses from the different feedbacks are independent, which is a reasonable first-order approximation but not entirely true (Soden et al., 2008).

2.2.3. Equilibrium and Effective Climate Sensitivity

An important metric describing climate sensitivity is the Equilibrium Climate Sensitivity. It is defined as the change in GSAT after an instantaneous doubling of the atmospheric CO_2 concentration from pre-industrial conditions once the climate system reaches radiative equilibrium (Bindoff et al., 2013). Being already used in one of the first assessments of the anthropogenic climate change, the *Charney Report* from 1979 (Charney et al., 1979), the Equilibrium Climate Sensitivity is one of the oldest metrics describing climate change. However, in practice this traditional definition of is not useful. Running fully-coupled ESMs into equilibrium is computationally expensive as it would require thousands of model years (M. Rugenstein et al., 2020).

For this reason, the Equilibrium Climate Sensitivity is commonly approximated with the Effective Climate Sensitivity (ECS), which can be derived from only 150 model years of a simulation with an abrupt quadrupling of the atmospheric CO_2 concentration ($4\times\text{CO}_2$) (Gregory et al., 2004). The basis of the definition of ECS is the simple energy balance model introduced in section 2.2.2. Assuming radiative equilibrium ($N = 0$), equations (2.1) and (2.6) imply

$$\Delta T = -\frac{F}{\lambda}. \quad (2.8)$$

Thus, the change in GSAT in radiative equilibrium can be easily calculated from the external forcing F and the climate feedback parameter λ . The steady state values for F and λ can be estimated from a $4\times\text{CO}_2$ simulation that is not in equilibrium by extrapolation with a linear regression (Gregory et al., 2004). For this method, the so-called *Gregory regression*, the global and annual mean net TOA radiation N vs. the change in the annual mean GSAT ΔT for

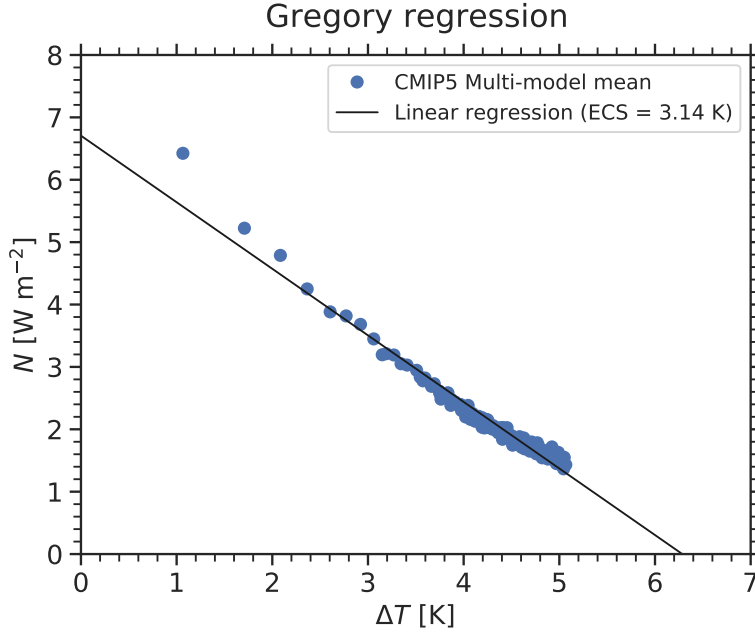


Figure 2.5.: Global and annual mean net top of the atmosphere (TOA) radiation N vs. the change in global and annual mean near-surface air temperature ΔT for 150 years of a simulation with an abrupt quadrupling of the atmospheric CO_2 concentration ($4\times\text{CO}_2$) for the CMIP5 multi-model mean (blue circles). To account for energy leakage and model drift, a linear fit of the corresponding pre-industrial control run is subtracted from the $4\times\text{CO}_2$ simulation. As given by equation (2.9), the slope of the linear regression (black line) corresponds to the climate feedback parameter λ and the y-intercept corresponds to the radiative forcing F_{4x} . These can be used to calculate the Effective Climate Sensitivity (ECS) with the Gregory regression method according to equation (2.10) (Gregory et al., 2004). ECS is equivalently given by the x-intercept of the linear regression line divided by 2. Here, $\text{ECS} = 3.14$ K.

all 150 years of the $4\times\text{CO}_2$ run are plotted (see figure 2.5). To account for energy leakage and remove any model drift present in the control climate, a linear fit of the corresponding pre-industrial control run is subtracted from the $4\times\text{CO}_2$ simulation beforehand (Andrews et al., 2012). Since the combination of equations (2.1) and (2.6) yields

$$N = F + \lambda \cdot \Delta T, \quad (2.9)$$

F is now given by the y-intercept of this linear regression (F_{4x}) and λ by its slope. Thus, the ECS is given by

$$\text{ECS} = -\frac{F_{4x}}{2\lambda}. \quad (2.10)$$

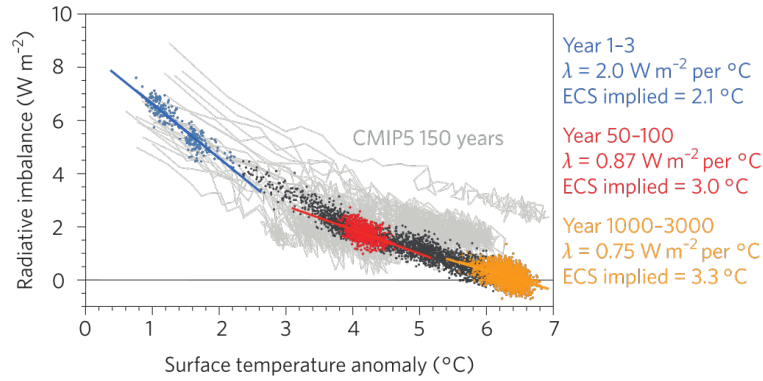


Figure 2.6.: As figure 2.5, but for different time periods considered in the Gregory regression resulting in different values for the Effective Climate Sensitivity (ECS) and the climate feedback parameter λ . Dark gray, blue, red and orange colors correspond to the Community Earth System Model (CESM) of the National Center for Atmospheric Research (NCAR) for different time periods of a long running simulation (see legend). The initial years are simulated many times for different initial conditions. Light gray colors correspond to the CMIP5 ensemble (150 years each). Taken from Knutti, Rugenstein, and Hegerl (2017).

The factor of 2 in the denominator accounts for the fact the traditional Equilibrium Climate Sensitivity is defined for an abrupt CO_2 doubling, whereas here a simulation with an abrupt quadrupling is considered.

Although commonly used in the literature, the ECS is known to be only an approximation of the true Equilibrium Climate Sensitivity. One major reason for this is the state and time dependence of the global feedbacks (Knutti, Rugenstein, & Hegerl, 2017; Knutti & Rugenstein, 2015). As figure 2.6 shows, the slope in the Gregory regression is not constant, but rather decreases over time when a long running $4\times\text{CO}_2$ simulation with more than 1000 model years is considered. As a result, the climate feedback parameter λ decreases over time, resulting in a higher ECS. Major reasons for this are temperature dependencies of the feedbacks, atmospheric and oceanic adjustments over time, changing warming patterns over time, non-additive feedbacks and dependencies on the type and magnitude of the external forcings (Knutti, Rugenstein, & Hegerl, 2017). All in all, this demonstrates the limits of the linear feedback framework introduced in section 2.2.2 that is not capable of describing non-linear effects. A second major reason for the discrepancies between the Equilibrium Climate Sensitivity and ECS is the use of a $4\times\text{CO}_2$ instead of a $2\times\text{CO}_2$ simulation. The factor of 2 in the denominator of equation (2.10) only partly compensates this difference since the radiative forcing logarithmically depends on the atmospheric CO_2 concentration (Huang & Shahabadi, 2014).

However, despite these deficiencies the ECS is still a practical estimate of the Equilibrium Climate Sensitivity. With the help of climate models, Sherwood et al. (2020) showed that the ECS is only about 6 % lower than the best estimate of the true equilibrium warming obtained from integrating climate models until a new steady state is reached. Nevertheless, for CMIP6 long running simulations from the Long Run Model Intercomparison Project (LongRunMIP) (M. Rugenstein et al., 2019) can be a promising way forward to estimate the true Equilibrium Climate Sensitivity for ESMs.

2.2.4. Transient Climate Response

A further metric describing the climate sensitivity is the Transient Climate Response (TCR). In contrast to the ECS, this metric does not assume radiative equilibrium of the Earth system but describes the transient response of an evolving climate. Following Bindoff et al. (2013), TCR is defined as the change in the GSAT at the time of CO₂ doubling in a simulation with a 1 % per year increase of the atmospheric CO₂ concentration (1%CO₂). For this, the annual mean GSATs are averaged over a 20 year period centered at the time of the CO₂ doubling (years 61–80 when the first year is indexed with 1). To account for model drift, the annual mean changes in GSAT are calculated relative to a corresponding pre-industrial control simulation smoothed with a linear fit that considers 140 model years (length of the 1%CO₂ simulation). An illustration of that calculation is shown in figure 2.7.

Similar to ECS, TCR can also be defined in terms of an external forcing and climate feedbacks. For this, the energy balance equation (2.9) can be slightly adjusted. Since over 90 % of the excess energy introduced into the climate system by the radiative forcing F is taken up by the ocean due to its large heat capacity, N can be taken equal to the global ocean heat uptake (Knutti, Rugenstein, & Hegerl, 2017). In experiments with a steadily increasing radiative forcing, which is the case for the 1%CO₂ simulation, this ocean heat uptake can be approximated with

$$N = \kappa \cdot \Delta T, \quad (2.11)$$

where κ is the ocean heat uptake efficiency (Gregory & Forster, 2008). Since there is a net energy flux into the climate system ($N > 0$) due to the external forcing F , κ is positive. This approximation becomes less accurate as the deeper ocean warms up and cannot be applied to simulations with a steady state climate change ($N \rightarrow 0$) where the external forcing tends stabilize (Gregory et al., 2009).

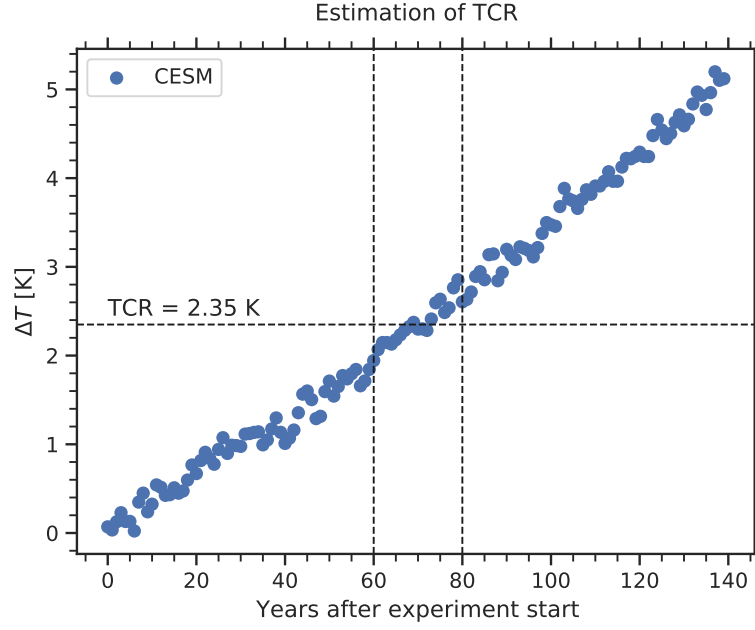


Figure 2.7.: Global and annual mean near-surface air temperature change ΔT for 140 years of a simulation with a 1 % per year increase of the atmospheric CO_2 concentration (1% CO_2) for the Community Earth System Model (CESM) of the National Center for Atmospheric Research (NCAR) (blue circles). The temperature change is calculated relative to a corresponding pre-industrial control simulation smoothed with a linear fit over all 140 years. The Transient Climate Response (TCR) is defined as the temperature change ΔT at the time of CO_2 doubling averaged over a 20 year period (illustrated by the vertical dashed lines). Here, $\text{TCR} = 2.35 \text{ K}$ (horizontal dashed line).

By applying the definition of TCR (transient GSAT change ΔT at the time of CO_2 doubling) and combining equations (2.9) and (2.11), TCR can be estimated as

$$\text{TCR} = \frac{F_{2x}}{\kappa - \lambda}, \quad (2.12)$$

where F_{2x} is the radiative forcing induced by a doubling of the atmospheric CO_2 concentration.

This equation can be used to derive a relationship between TCR and ECS. Writing $\text{ECS} = -F_{2x}/\lambda$ and assuming path independence of the forcing (i.e. the resulting radiative forcing from the 1% CO_2 and 2x CO_2 runs are comparable) gives

$$\text{TCR} = \frac{F_{2x} \cdot \text{ECS}}{F_{2x} + \kappa \cdot \text{ECS}}, \quad (2.13)$$

which demonstrates the non-linear connection between TCR and ECS (Gregory & Forster, 2008; Nijse et al., 2020). Since $\lambda < 0$ and $\kappa > 0$, equation (2.12) implies that the equilibrium response ECS is (as expected) larger than transient response TCR, i.e. $\text{ECS} > \text{TCR}$.

2.3. The Global Carbon Cycle

Since one study presented in this thesis aims to reduce uncertainties in carbon cycle-related processes (Schlund, Eyring, et al., 2020; see chapter 6), this chapter introduces the scientific background of the global carbon cycle.

2.3.1. Overview

A schematic overview of the global carbon cycle is shown in figure 2.8. To quantify the carbon cycle, common units are parts per million (ppm) for the atmospheric trace gas concentrations (dry-air mole fraction) and gigatonnes of carbon (GtC) or GtC yr^{-1} for the reservoirs masses or exchange fluxes, respectively. The carbon exchange processes between the different carbon reservoirs run on a wide range of time scales. Conceptually, one can distinguish between two domains of the global carbon cycle: a slow and a fast domain. The slow domain with turnover times (reservoir mass of carbon divided by exchange flux) of more than 10000 years consists of the large carbon stores in rocks and sediments which are connected to the rapid domain of the carbon cycle through volcanic emissions of CO_2 , chemical weathering, erosion and sediment formation on the sea floor. These natural exchange fluxes between the slow and the fast domain are comparatively small ($< 0.3 \text{ GtC yr}^{-1}$) and can be assumed as approximately constant in time over the last few centuries (Ciais et al., 2013).

The fast domain of the global carbon cycle consists of three main carbon reservoirs: the atmosphere, the terrestrial biosphere and the ocean. In the atmosphere, carbon is mainly stored in trace gases, with CO_2 as the major component with a current (2019) concentration of about 410 ppm (Friedlingstein et al., 2019). Additional contributors to the atmospheric carbon content are the trace gas methane (CH_4), the trace gas carbon monoxide (CO), hydrocarbons, black carbon aerosols and organic compounds (Ciais et al., 2013). Carbon in the terrestrial biosphere is mainly stored as organic compounds, with about 450–650 GtC in the living vegetation biomass, 1500–2400 GtC in dead organic matter in litter and soils and about 1700 GtC in permafrost soils (Ciais et al., 2013). The main component of the oceanic carbon reservoir is dissolved inorganic carbon (carbonic acid, bicarbonate ions and carbonate ions) with about 38000 GtC. Further carbon is stored as dissolved organic carbon (about 700 GtC), in surface sediments (about 1750 GtC) and in marine biota (about 3 GtC, predominantly phytoplankton and other microorganisms) (Ciais et al., 2013; Friedlingstein et al., 2019).

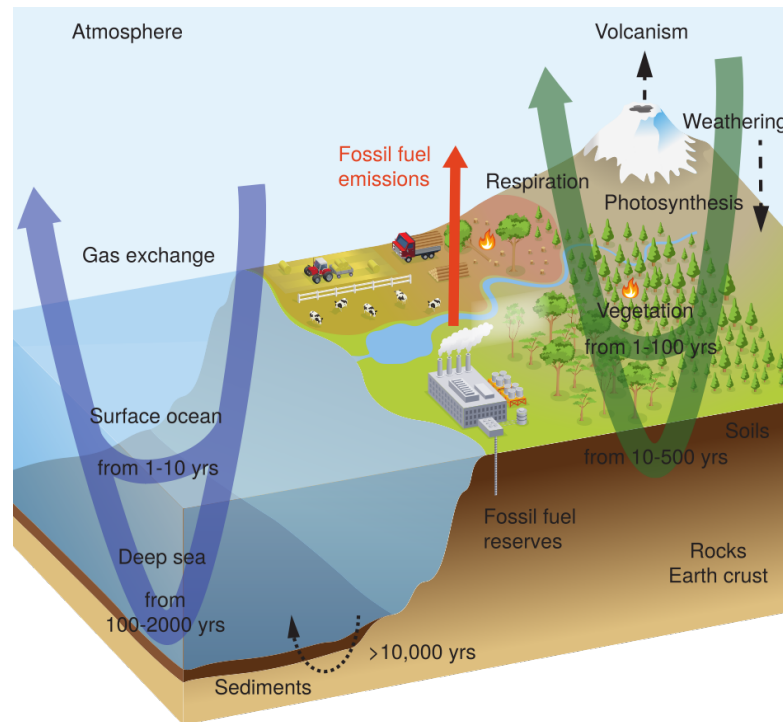


Figure 2.8.: Simplified schematic of the global carbon cycle including the typical turnover time scales for carbon transfers through the major reservoirs (atmosphere, land surface and ocean). Taken from Ciais et al. (2013).

In the fast domain of the global carbon cycle, reservoir turnover times range from seconds to millennia. In contrast to the slow domain, the carbon exchange fluxes within the fast domain of the carbon cycle are much higher. One major group of exchange processes in the fast domain connects the atmosphere and the terrestrial biosphere. CO₂ is removed from the atmosphere by plant photosynthesis with about 120 GtC yr⁻¹ (Ciais et al., 2013). This process is also known as Gross Primary Productivity (GPP). The carbon fixed into plants can be released back into the atmosphere by autotrophic (plant) and heterotrophic (soil microbial and animal) respiration and additional disturbance processes like fires (Ciais et al., 2013). Since the land CO₂ uptake by photosynthesis occurs only during the growing season, whereas respiration occurs nearly all year, the larger amount of vegetation in the Northern hemisphere (due to the larger land mass) gives rise to a seasonal cycle of the atmospheric CO₂ concentration (Keeling et al., 1995). This seasonal cycle reflects the phase of the global carbon cycle and shows a maximum of the atmospheric CO₂ concentration in the Northern hemisphere winter (net CO₂ flux into atmosphere due to respiration) and a minimum during the Northern hemisphere summer (net CO₂ flux into the land due to photosynthesis). Another major carbon exchange process connects the atmosphere and the ocean. Atmospheric CO₂ is exchanged with the surface ocean

through gas exchange, which is driven by the partial CO₂ pressure difference between the air and the sea (Ciais et al., 2013).

2.3.2. Anthropogenic Perturbations

Before the Industrial Era, the global carbon cycle was roughly in a dynamic equilibrium, which means that exchange fluxes balanced each other and the amount of carbon in the different reservoirs did neither increase nor decrease. This can be inferred from ice core measurements, which show an almost constant atmospheric CO₂ concentration over the last several thousand years before the Industrial Revolution in the 19th century (Ciais et al., 2013). Since the beginning of the Industrial Era, humanity is constantly emitting carbon-based GHGs (e.g. CO₂ and CH₄) into the atmosphere. Especially the atmospheric CO₂ concentration has substantially increased, which has already been shown by Charles D. Keeling in 1976 by his continuous CO₂ measurements at Mauna Loa, Hawaii that started in 1958 (Keeling et al., 1976; see figure 2.9). From 1958, the atmospheric CO₂ concentration at Mauna Loa has steadily increased by about 100 ppm to 410 ppm in the year 2019 (Keeling et al., 2005). In addition to the steady increase, the so-called *Keeling Curve* is further superimposed with the seasonal CO₂ cycle, which gives rise to local maxima of the atmospheric CO₂ concentration in the Northern hemisphere winter and local minima in the Northern hemisphere summer (Keeling et al., 1995; see section 2.3.1). Due to its location in the middle of the Pacific Ocean, the Mauna Loa Observatory offers perfect conditions for CO₂ measurements by being far away from big population centers. Moreover, its elevation of more than 3000 m provides access to the well-mixed air of the Pacific Ocean in high altitudes, which prevents any interference from the vegetation present on the Hawaiian Islands.

Apart from warming the Earth by altering its radiation budget, the anthropogenically emitted CO₂ directly influences the carbon exchange fluxes of the global carbon cycle. Due to the excessive carbon in the atmosphere, there is now a net carbon flux from the atmosphere into the land and ocean reservoirs (see figure 2.10). Thus, the carbon cycle is not in a steady state anymore. In the decade 2009–2018, anthropogenic activities caused net carbon fluxes of 3.2 GtC yr⁻¹ from the atmosphere into the terrestrial biosphere due to increased plant photosynthesis and 2.5 GtC yr⁻¹ from the atmosphere into the ocean due to increase dissolution of CO₂ into the sea (Friedlingstein et al., 2019). In the same time, the amount of carbon in the atmosphere reservoir increased with a rate of 4.9 GtC yr⁻¹, indicating that only about half of the anthropogenic CO₂

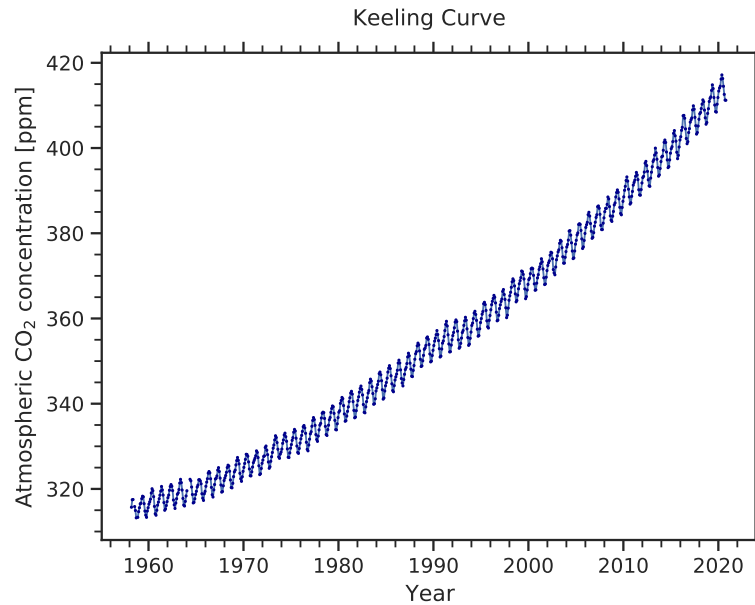


Figure 2.9.: The Keeling Curve: monthly-mean atmospheric CO₂ concentration at the Mauna Loa Observatory, Hawaii (19.5°N, 155.6°W; elevation: 3397 m) from 1958 to 2019 (Keeling et al., 2005). The steady increase of the atmospheric CO₂ concentration is superimposed with a seasonal oscillation caused by the seasonal CO₂ cycle (see section 2.3.1).

emissions in the last decade remained in the atmosphere (Friedlingstein et al., 2019) where they can act as GHG.

Thus, this removal of CO₂ from the atmosphere actively slows down global warming. However, whether this benefit will persist in the future remains unclear, which is primarily linked to two feedback processes connecting the physical climate system and the global carbon cycle: the *concentration-carbon feedback* and the *climate-carbon feedback* (M. Collins et al., 2013; Friedlingstein et al., 2006; Gregory et al., 2009). For the terrestrial biosphere, the concentration-carbon feedback is connected to the *CO₂ fertilization effect* (Walker et al., 2020), that causes an increase of photosynthesis rates when the atmospheric CO₂ concentration increases, which in turns removes CO₂ from the atmosphere, forming a negative feedback. For the ocean, the concentration-carbon feedback is negative as well. In this case, an elevated atmospheric CO₂ concentration causes an increased dissolution of CO₂ into the sea, which increases the ocean carbon uptake. On the other hand, the climate-carbon feedback is thought to be positive for both the terrestrial biosphere and the ocean (Gregory et al., 2009). In the first case, temperature and precipitation changes due to anthropogenic activities decrease the land carbon uptake because of increased temperature and water stress on photosynthesis and higher ecosystem respiration costs, which

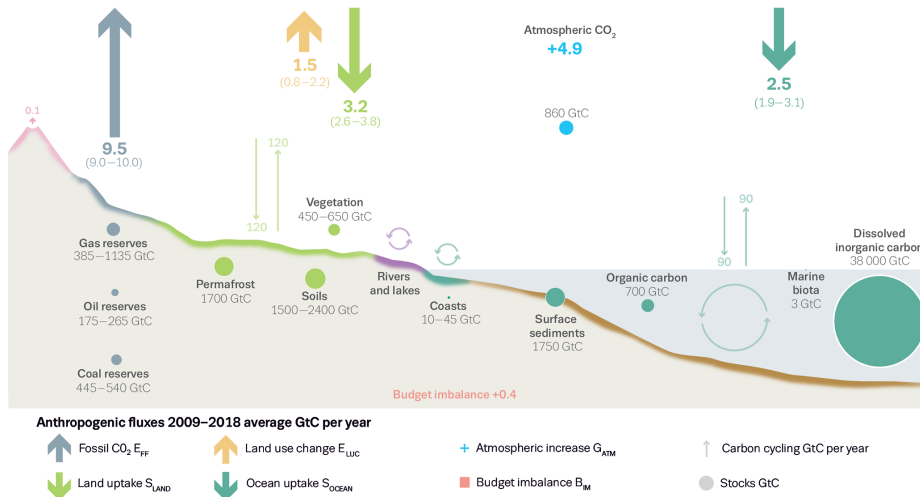


Figure 2.10.: Schematic representation of the overall perturbation of the global carbon cycle caused by anthropogenic activities, averaged globally for the decade 2009–2018. Arrows represent carbon exchange fluxes; circles carbon reservoirs. More details are given in the legend of this figure. Taken from Friedlingstein et al. (2019).

accelerates global warming due to more CO₂ that remains in the atmosphere. For the ocean, increased temperatures lead to a reduction of vertical transport in the ocean resulting from increased stability and reduced solubility of CO₂ in the sea, which reduces the ocean carbon uptake and enhances climate change (Gregory et al., 2009).

2.4. Reducing Uncertainties in Multi-Model Climate Projections with Observations

As shown in section 2.1.3, projections of the future climate are always associated with uncertainties. In the context of this thesis, the most relevant source of uncertainty is the climate response uncertainty. It originates from our imperfect knowledge on how the climate system will respond to external forcing. In a multi-model ensemble (e.g. from CMIP), this is expressed as the different responses of the different climate models to a given forcing. A common approach to distill information about a projected quantity from multi-model ensembles is to treat the arithmetic multi-model mean (MMM) and the multi-model range as best estimate and uncertainty measure of this quantity (M. Collins et al., 2013). This *model democracy* approach basically assumes that all climate models are independent, equally plausible, distributed around reality and that the projected multi-model range is representative for the uncertainty in the projected quantity

(Knutti, Sedlacek, et al., 2017). However, since the CMIP ensembles, sometimes referred to as *ensembles of opportunity*, have not been designed to represent a true statistical sample of the reality composed of independent climate models (Tebaldi & Knutti, 2007), these assumptions do not hold in practice. The main reasons for this are that different climate models (even for different modeling institutions) share parts of their code (Abramowitz et al., 2019; Knutti et al., 2013), that models do not equally well represent the observed past and present-day climate (Gleckler et al., 2008; Knutti et al., 2013) and that models might suffer from common structural limitations like missing processes (Knutti, Sedlacek, et al., 2017).

Thus, more sophisticated techniques are necessary to evaluate multi-model climate projections. This section introduces three state-of-the-art methods to assess multi-model projections and reduce associated uncertainties with observations. These techniques form the baseline of the work presented in the following chapters.

2.4.1. Emergent Constraints

As indicated at the beginning of this section, one main issue of multi-model ensembles is that not all participating climate models are equally plausible. Usually, this is quantified with some kind of measure of the models' *performance*, i.e. their agreement with observations of the real climate system. However, this model performance can only be evaluated against observations of the past and present-day climate, which does not necessarily provide insights into the quality of model projections of the future climate.

The *emergent constraint* approach tackles this problem by “identifying robust, physically interpretable relationships between Earth system feedback behaviors on short, well-observed time scales and on time scales that span the twenty-first century and beyond” (Eyring et al., 2019). An illustration of the concept of emergent constraints is shown in figure 2.11. Each emergent constraint requires two key components: an *emergent relationship* and a corresponding observation of the real world (Eyring et al., 2019). The emergent relationship (red line in figure 2.11) is a robust and physically interpretable inter-model relationship between a target variable y related to the future climate and an observable x of the past or present-day climate. Basis for the relationship is output of the different climate models of a multi-model ensemble (blue circles in figure 2.11). Using an observation of x , this emergent relationship can then be used to derive a emergent constraint on y (gray shaded area in figure 2.11) that considers

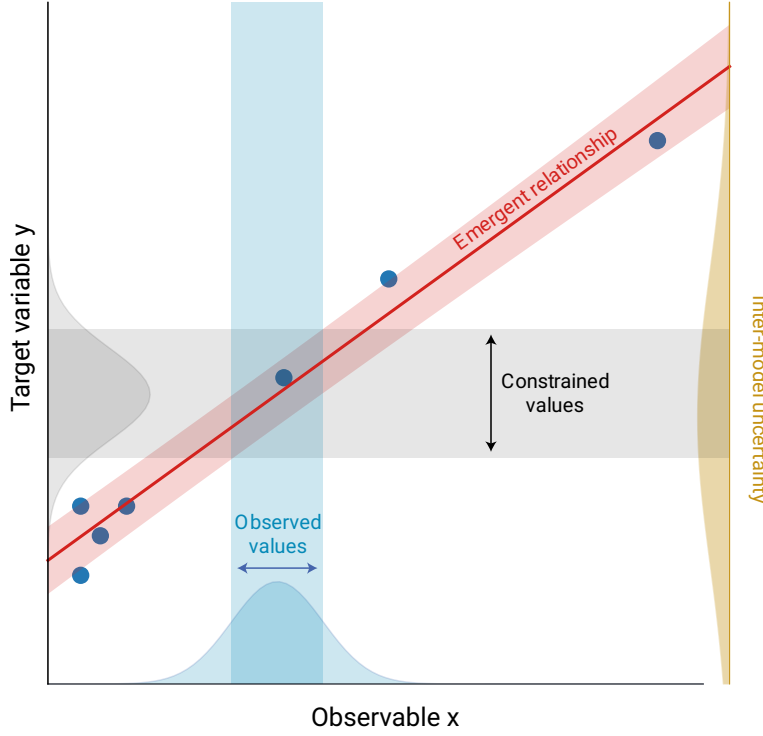


Figure 2.11.: Schematic illustration of the emergent constraint approach. Basis of every emergent constraint is a robust and physically interpretable emergent relationship (red line) between a target variable y (e.g. Earth system sensitivity or projection of future climate change) and an observable x (e.g. past or present-day trend or variation) for the climate models of a multi-model ensemble (blue circles). With an observation of x , uncertainties in y in the multi-model ensemble, illustrated by the yellow probability density function (PDF), can be reduced (gray PDF). Uncertainties in the target variable y arise from two sources: uncertainties in the observation (blue shaded area) and uncertainties in the emergent relationship (red shaded area). Taken and modified from Eyring et al. (2019).

uncertainties in the emergent relationship itself (red shaded area in figure 2.11) and uncertainties in the observation (blue shaded area in figure 2.11).

One possible mathematical framework for the evaluation of emergent constraints is based on linear regression and Gaussian probability densities (Cox et al., 2018; Cox et al., 2013). Let x_m be the observable predictor variable for climate model m and y_m the corresponding target variable. To find the linear emergent relationship for a climate model ensemble with M climate models and data $\{(x_m, y_m) \mid m \in I_M\}$ with index set $I_M = \{1, 2, \dots, M\}$, a linear regression model

$$\hat{y}(x) = \hat{b}_0 + \hat{b}_1 x \quad (2.14)$$

for the predicted target variable \hat{y} with estimated intercept \hat{b}_0 and slope \hat{b}_1 is used (see equation (2.25) for details on this). Fitting this regression line with ordinary least squares includes minimizing the standard error s of the estimate

$$s^2 = \frac{1}{M-2} \sum_{m=1}^M (y_m - \hat{y}_m)^2, \quad (2.15)$$

where $\hat{y}_m := \hat{y}(x_m)$ is the predicted target variable for climate model m and M is the total number of climate models. The uncertainty of the emergent relationship for a value x that has not been used to fit the regression line is given by the standard prediction error $\sigma_{\hat{y}}(x)$:

$$\sigma_{\hat{y}}^2(x) = s^2 \left[1 + \frac{1}{M} + \frac{(x - \bar{x})^2}{\sum_{m=1}^M (x_m - \bar{x})^2} \right]. \quad (2.16)$$

Here, \bar{x} indicates the arithmetic mean of x over all climate models. Assuming Gaussian errors and a mean of $\hat{y}(x)$ (i.e. the best estimate of the target variable y is given by the regression line), equation (2.16) can be used to define a conditional probability density function (PDF) for predicting a target variable of y given x :

$$P(y|x) = \frac{1}{\sqrt{2\pi\sigma_{\hat{y}}^2(x)}} \exp \left[-\frac{(y - \hat{y}(x))^2}{2\sigma_{\hat{y}}^2(x)} \right]. \quad (2.17)$$

This distribution describes the uncertainty in the emergent relationship itself introduced by the imperfect alignment of the climate model data (red shaded area in figure 2.11). Its maximum is given by the emergent relationship itself (red line in figure 2.11). The conditional PDF can be interpreted as the posterior distribution of the regression model based on the climate model output but constrained on the observable x . However, the observed value of x , called x_0 , also has uncertainties associated with it (blue shaded area in figure 2.11). Assuming again a Gaussian distribution, the observational PDF for observing x_0 given the true value x can be written as

$$P(x_0|x) = \frac{1}{\sqrt{2\pi\sigma_x^2}} \exp \left[-\frac{(x_0 - x)^2}{2\sigma_x^2} \right], \quad (2.18)$$

where σ_x is the standard deviation of the observation around the true value. Assuming an imperfect uniform prior $P(x) \propto 1$ with cut-offs at $-\infty$ and $+\infty$ and using Bayes' theorem implies $P(x_0|x) = P(x|x_0)$. In a final step, this can be used to calculate the posterior PDF for the constrained prediction of the target

variable y given the observation x_0 (gray PDF in figure 2.11) with numerical integration:

$$P(y|x_0) = \int_{-\infty}^{+\infty} P(y|x) P(x|x_0) dx. \quad (2.19)$$

Posterior estimates of the target variable are influenced by the way the statistical inference has been performed. Alternative methods that can be used include Bayesian frameworks (Renoult et al., 2020), information theoretic approaches based on the Kullback–Leibler divergence between the models’ PDFs of x and the observational PDF (Brient & Schneider, 2016) and linear regression models based on hierarchical Bayesian models (Nijssse et al., 2020). However, no consensus has yet been found for this statistical inference (Brient, 2020).

A convenient metric to quantify the skill of an emergent relationship is the coefficient of determination R^2 of its underlying statistical model. In the presented framework which is based on univariate ordinary least squares regression, R^2 is given by the squared Pearson correlation coefficient r evaluated on the climate model ensemble data $\{(x_m, y_m) \mid m \in I_M\}$, i.e. $R^2 = r^2$. A further quantity describing the skill of an emergent relationship is its statistical significance. In the introduced framework, a two-sided t -test can be used to determine how likely the correlation found between the target variable y and the predictor x would be to appear by chance. The null hypothesis for this test is that the predictor and the target variable are not linearly correlated, i.e. that the true underlying Pearson correlation coefficient of the population is zero. If this null hypothesis is true, the probability distribution of the variable

$$t = \frac{r\sqrt{M-2}}{\sqrt{1-r^2}} \quad (2.20)$$

is a Student’s t -distribution with $M - 2$ degrees of freedom. The statistical significance can then be measured with the p -value of this two-sided t -test, which describes the probability of obtaining an absolute sample Pearson correlation coefficient greater than $|r|$ if the null hypothesis is true. Smaller p -values indicate higher a higher statistical significance and vice versa.

One limitation of the presented framework is the assumption that the individual data points from the different climate models are independent. As already noted in the beginning of section 2.4, this is not the case for typical climate models ensembles, as some modeling groups provide output for multiple climate models and some climate models from different modeling institutions share components and code (Knutti et al., 2013). The duplicated code in the different climate models leads to an overestimation of the sample size and may result in

spurious correlations (Sanderson et al., 2015a). Possible approaches to tackle this problem are presented in section 2.4.2 and include a weighting of the climate models based on their degree of interdependence (Knutti, Sedlacek, et al., 2017; Sanderson et al., 2015a; Sanderson et al., 2017). A further limitation of this approach is the use of an ordinary least squares linear regression model. This is not always appropriate, for example when a non-linear emergent relationship is expected (Nijse et al., 2020) or when additional physical considerations further constrain the regression model, e.g. by demanding a zero intercept ($\hat{b}_0 = 0$) (Annan et al., 2020; Jimenez-de-la-Cuesta & Mauritsen, 2019). Moreover, using only a single observational dataset to estimate x_0 and σ_x when different datasets are available might lead to an underestimation of the observational uncertainty, as different observational datasets might lead to different emergent constraints.

A crucial aspect for every emergent constraint is a verifiable physical process explaining the correlation between x and y (Hall et al., 2019). Only if the underlying emergent relationship can be derived from a robust and plausible physical mechanism, an emergent constraint can be considered credible. The reason for this are spurious relationships: Due to the large number of possible observables provided by modern ESMs and the comparatively small number of climate models, spurious relationships are possible just by chance (Caldwell et al., 2014). Furthermore, out-of-sample tests offer an important tool to evaluate the credibility of emergent constraints (Hall et al., 2019). These ensure that the existence of an emergent relationship is not limited to a certain climate model ensemble and might indicate that the relationship is also valid for the true climate system. Testing emergent constraints in different CMIP generations offers a straightforward setup for out-of-sample testing (Caldwell et al., 2018), which is discussed in more detail in chapter 5, where eleven emergent constraints on ECS are evaluated on the new CMIP6 ensemble.

In the last two decades, many emergent constraints on various aspects of the Earth system have been published. Early studies tackled the hydrological cycle (Allen & Ingram, 2002) and the snow-albedo feedback (Hall & Qu, 2006). Over the years, the climate sensitivity expressed by the ECS has been a prominent target variable. Since cloud feedbacks are a major source of uncertainty for climate sensitivity, a variety of papers focus on constraining ECS with cloud-related processes (Brient & Schneider, 2016; Brient et al., 2015; Fasullo & Trenberth, 2012; Lipat et al., 2017; Qu et al., 2013; Sherwood et al., 2014; Su et al., 2014; Tian, 2015; Volodin, 2008; Zhai et al., 2015), which are discussed in detail in section 5.1. More recent studies aim to constrain ECS with the historical temperature variability (Cox et al., 2018) or the historical warming trend (Jimenez-de-la-Cuesta

& Mauritsen, 2019; Nijssen et al., 2020; Tokarska et al., 2020). Emergent constraints are not only limited to physical processes, but can also be applied to other domains, like the global carbon cycle (Cox et al., 2013; Kwiatkowski et al., 2017; Wenzel et al., 2014, 2016; Winkler et al., 2019). An extensive discussion on the emergent constraint by Wenzel, Cox, et al. (2016), which focuses on the concentration-carbon feedback, is given in section 6.1.

2.4.2. Performance- and Interdependence-based Weighting of Climate Models

A further technique to reduce uncertainties in climate model projections with observations are model weighting schemes. Their basic idea is to abandon model democracy by replacing the arithmetic mean used to calculate the MMMs by a weighted mean of the form

$$y = \sum_{m=1}^M w_m y_m \quad (2.21)$$

with normalized weights w_m . Similar to the notation introduced in the previous section, y is a target variable (e.g. a projection of the future climate) and m indexes the M different climate models. To address two major issues of model democracy (different climate models are not equally plausible and not independent; see beginning of section 2.4), Knutti, Sedlacek, et al. (2017) propose a weighting scheme based on climate model performance and interdependence with the following weights:

$$w_m \propto \frac{\exp\left(-\frac{D_m^2}{\sigma_D^2}\right)}{1 + \sum_{n \neq m}^M \exp\left(-\frac{S_{mn}^2}{\sigma_S^2}\right)}. \quad (2.22)$$

The metric D_m describes the distance between climate model m and observations (= model performance) and the metric S_{mn} describes the distance between climate model m and n (= model interdependence). σ_D and σ_S are constants that determine the individual strength of the performance and interdependence weighting, respectively.

A commonly used distance metric to measure model performance D_m and model interdependence S_{mn} is the root-mean-square error (RMSE), but others are possible (Knutti, Sedlacek, et al., 2017). The metrics are evaluated on a set of past or present-day diagnostics and variables, whose choice is crucial for the weighting scheme. A helpful strategy for this is to focus on addressing the question “which climate model is adequate for predicting the target variable

y ?” instead of trying to answer the question “which climate model is the best?” (Parker, 2009). Thus, diagnostics and variables are chosen that are relevant for the projection of the target variable (Knutti, Sedlacek, et al., 2017). In practice, this choice is either based on expert judgment about relevant processes, on emergent relationships (see section 2.4.1) or on multivariate regression models (Karpechko et al., 2013; Sanderson et al., 2015b; see section 2.4.3). It might also be beneficial to use different diagnostics for the calculations of the performance and interdependence metrics (Merrifield et al., 2020) and/or to remove selected diagnostics based on their mutual correlation (Lorenz et al., 2018).

The constants σ_D and σ_S determine how strongly the climate models’ performance and interdependence are weighted (Knutti, Sedlacek, et al., 2017). Small values of the performance parameter σ_D lead to an aggressive weighting with only a few climate models receiving a majority of the weight, while large values of σ_D result in an equal weighting. For the interdependence parameter σ_S , this is slightly different: Here, small (all climate models are independent) and large (all climate models are dependent) values lead to an almost equal weighting. Thus, an optimal choice for σ_D and σ_S is crucial. A useful tool to estimate these optimal parameters is the *leave-one-model-out cross-validation* (CV) approach, which is also known as *pseudo-reality*, *model-as-truth* or *perfect model* setup (de Elia et al., 2002; Karpechko et al., 2013). For this, a single climate model is removed from the multi-model ensemble and treated as observation (*pseudo-observation*). Then, a weighted MMM with weights computed from the updated model ensemble is calculated, which gives a prediction for the “true” climate model. This allows a simple quantitative assessment of the weighting scheme by calculating the RMSE between the prediction and the known ground truth of the pseudo-observation. The whole process is repeated for every climate model of the ensemble to get a statistical distribution of RMSEs. Finally, different RMSE distributions calculated from different parameters σ_D and σ_S can be assessed using specific criteria to find optimal values for σ_D and σ_S (Knutti, Sedlacek, et al., 2017). Furthermore, the leave-one-model-out CV approach can be used to evaluate different climate model weightings schemes (including the unweighted MMM) and compare them against each other.

The definition of the weights according to equation (2.22) is based on reasonable and comprehensible principles. However, the exact form of the equation is purely subjective. Moreover, the additional freedom in choosing a suitable metric and optimal values for the parameters σ_D and σ_S adds another level of subjectivity to the weighting scheme, which can partly be addressed with the introduced leave-one-model-out CV setup. Nevertheless, due to its flexibility,

the climate model weighting scheme of Knutti, Sedlacek, et al. (2017) has already been used for various target variables: Arctic sea ice (Knutti, Sedlacek, et al., 2017), Antarctic ozone concentrations (Amos et al., 2020), North American maximum temperature (Lorenz et al., 2018), European temperature and precipitation (Brunner et al., 2019; Merrifield et al., 2020) and global warming over the 21st century (Brunner et al., 2020; Liang et al., 2020).

2.4.3. Multiple Diagnostic Ensemble Regression

An alternative climate model weighting scheme is the *Multiple Diagnostic Ensemble Regression (MDER)* approach (Karpechko et al., 2013). Similar to all methods presented in section 2.4, it can be used to reduce uncertainties in climate model projections with observations. The basis of MDER is a set of K predictor diagnostics $\{x^{(1)}, x^{(2)}, \dots, x^{(K)}\}$ which are relevant for the projection of the target variable y . The reasoning for this choice of the diagnostics is similar to the one presented in the previous section: Weighting schemes should address the question “which climate model is adequate for predicting the target variable?” and not “which climate model is the best?”.

The concept of MDER is mathematically similar to the concept of emergent constraints. In a first step, an inter-model relationship between the target variable and the process-relevant diagnostics is used to fit a multivariate linear regression model. Let $\mathbf{y} = (y_1, y_2, \dots, y_M)^T \in \mathbb{R}^M$ be the vector of target variables of the M climate models (T denotes the transpose) and $\mathbf{X} \in \mathbb{R}^{M \times (K+1)}$ the design matrix representing the predictors:

$$\mathbf{X} = \begin{pmatrix} 1 & x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(K)} \\ 1 & x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(K)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_M^{(1)} & x_M^{(2)} & \dots & x_M^{(K)} \end{pmatrix}. \quad (2.23)$$

The entry $x_m^{(k)}$ of this matrix refers to the diagnostic variable of diagnostic k and climate model m . With this notation, the linear inter-model relationship can be written as

$$\mathbf{y} = \mathbf{X}\mathbf{b} + \boldsymbol{\varepsilon}, \quad (2.24)$$

where $\mathbf{b} = (b_0, b_1, \dots, b_K)^T \in \mathbb{R}^{(K+1)}$ is the vector of linear coefficients (with intercept b_0) and $\boldsymbol{\varepsilon} = (\varepsilon_1, \varepsilon_2, \dots, \varepsilon_M)^T \in \mathbb{R}^M$ a vector of independent random variables representing the noise in the target variable. Figure 2.12 shows a schematic that illustrates this linear relationship (gray surface) for the different

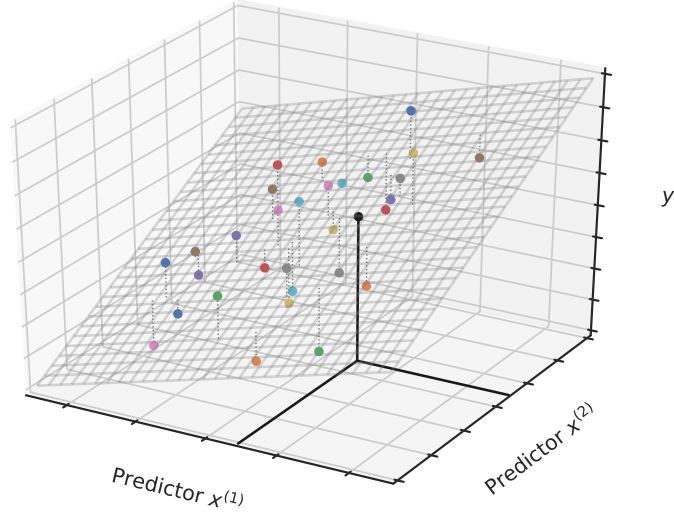


Figure 2.12.: Schematic illustration of the Multiple Diagnostic Ensemble Regression (MDER) approach (Karpechko et al., 2013). First, inter-model relationships between a target variable y and multiple process-based predictors $x^{(k)}$ (here: two predictors $x^{(1)}$ and $x^{(2)}$) are used to fit a multivariate linear regression model (gray surface). Second, observations of the predictors (horizontal black lines) are fed into the regression model to calculate an observation-based best estimate of the target variable \hat{y}_0 following equation (2.26). The black circle indicates the best estimate for the target variable y given by the observed values of $x^{(1)}$ and $x^{(2)}$. Each of the remaining colored circles represents a single climate model of the multi-model ensemble. The vertical dashed lines visualize the distance between the climate model data and the linear regression surface and represent the noise terms ε in equation (2.24).

climate models (colored circles) for two diagnostics ($K = 2$). Using ordinary least squares regression, the estimated linear coefficients $\hat{\mathbf{b}}$ are given by

$$\hat{\mathbf{b}} = \left(\mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{y}, \quad (2.25)$$

where the exponent -1 denotes the inverse matrix. Since this definition works for any number of diagnostics K , it can also be used to calculate the linear coefficients \hat{b}_0 (intercept) and \hat{b}_1 (slope) that define emergent relationships (see equation (2.14)).

In a second step, observed data of the process-based diagnostics $\mathbf{x}_0 = \left(1, x_0^{(1)}, x_0^{(2)}, \dots, x_0^{(K)} \right)^T \in \mathbb{R}^{(K+1)}$ is fed into the multivariate linear regression model to get an observation-based prediction of the target variable \hat{y}_0 (Karpechko et al., 2013):

$$\hat{y}_0 = \mathbf{x}_0^T \hat{\mathbf{b}} \quad (2.26)$$

This is mathematically similar to the calculation of the best estimate target variable y for emergent constraints. In figure 2.12, the observations of the predictors x_0 are illustrated with horizontal black lines and the best estimate \hat{y}_0 is shown as a black circle. By combining equations (2.25) and (2.26) and comparing this to the definition of weighted means in equation (2.21), climate model weights $w = (w_1, w_2, \dots, w_M)^T \in \mathbb{R}^M$ can be defined by

$$w = \left[x_0^T (X^T X)^{-1} X^T \right]^T, \quad (2.27)$$

which can be used to calculate the weighted target variable by

$$\hat{y}_0 = \hat{w}^T y. \quad (2.28)$$

A crucial aspect for the success of the MDER approach is the choice of the process-relevant diagnostics. In addition to the pre-selection based on expert judgment, an additional selection based on statistical criteria is necessary for two reasons: First, predictors which only show a weak correlation with the target variable should not be included in the regression model since they introduce additional noise and might lead to overconfident results. Second, multicollinearity (i.e. mutually correlated predictors) should be avoided since this reduces the robustness of the linear regression. A common technique to deal with these problems is a stepwise feature selection algorithm based on statistical tests of the correlations between the involved variables (Karpechko et al., 2013).

The basic assumption of the MDER algorithm is that the inter-model relationship between the process-based predictors and the target variable also holds for the true climate. This may seem weak at first glance, especially since it explicitly requires climate models that deviate from the observed climate to span the desired relationship (similar to emergent constraints). However, a much weaker assumption is made traditional in weighting approaches which assume that climate models that are better in simulating the past or present-day climate are necessarily better in simulating the future climate. In contrast to these other weighting approaches, MDER explicitly establishes the relationship between past/present and future within the climate model ensemble (Karpechko et al., 2013).

Drawbacks of the MDER approach are the missing consideration of errors in the observational data, the limitation to linear relationships between the process-relevant diagnostics and the target variable and the limitation to a single data point per climate model. Despite these, MDER has been successfully used to constrain uncertainties in Antarctic total ozone projections (Karpechko et al.,

2013), in the projected change of the austral jet position (Wenzel, Eyring, et al., 2016) and in projections of the Arctic sea ice extent (Senftleben et al., 2020).

3. Improving Routine Climate Model Evaluation

- overview ESMValTool
 - Changes in ESMValCore + table
 - Added recipes and diagnostics for ESMValTool + table
 - * Anav13
 - * MDER
 - * TCR
 - * ECS
 - * Schlund20jgr
 - * Schlund20ESD
 - * Flato13
 - total number of changed lines of code

4. Assessment of Policy-Relevant Climate Metrics in CMIP6

TBA.

5. Evaluation of Emergent Constraints on the Effective Climate Sensitivity in CMIP6

TBA.

5.1. Comparison of Emergent Constraints on ECS for CMIP5 and CMIP6

TBA.

6. Constraining Uncertainties in Future Gross Primary Productivity with Machine Learning

TBA.

6.1. Step 1: XXXXXXXXXXXXXXXXXXXXX

7. Summary and Outlook

TBA.

Appendix

A. TBA

A.1. test

test

hi The ECS is really cool. I like it very much!

This is e.g. without an "at" and this is it with an "at" e.g. difference? Test space. Real dot!

E.g. blaa. E.g. blaaaa. i.e. blaaaa, i.e. blaa.

These are really cool papers: (Schlund, Lauer, et al., 2020; Schlund, Eyring, et al., 2020)

autocite: (Lauer et al., 2018)

cite: Lauer et al., 2010 (Anav et al., 2015) (Anav et al., 2013) (Allen & Ingram, 2002)

textcite: Lauer et al. (2010)

And this one, too: (Lauer et al., 2020)

This is a reference to the equation: equation (1)

Three authors: (Bao et al., 2020)

Many many authors: (Eyring et al., 2020)

input <iostream>

$$c_{k_1, k_2} := 1200 \log_2 \left(\frac{f_1^{(k_2)}}{f_1^{(k_1)}} \right) \text{ cents.} \quad (1)$$

B. TBA

TBA.

Table 1.: The effects of treatments X and Y on the four groups studied.

Groups	Treatment X	Treatment Y
1	0.2	0.8
2	0.17	0.7
3	0.24	0.75
4	0.68	0.3

Semitones	Interval	c / cents (ET)	c / cents (JI)
0	Perfect unison	0	0
1	Minor second	100	112
2	Major second	200	204
3	Minor third	300	316
4	Major third	400	386
5	Perfect fourth	500	498
6	Augmented fourth	600	590
7	Perfect fifth	700	702
8	Minor sixth	800	814
9	Major sixth	900	884
10	Minor seventh	1000	996
11	Major seventh	1100	1088
12	Perfect octave	1200	1200

Table 2.: Logarithmic frequency ratios c of certain intervals in the equal temperament (ET) and the just intonation (JI). x cents correspond to a frequency ratio of $2^{x/1200}$.

List of Acronyms

AerChemMIP Aerosol Chemistry Model Intercomparison Project	6
AOGCM Atmosphere-Ocean General Circulation Model	3
C4MIP Coupled Climate-Carbon Cycle Model Intercomparison Project . .	6
CESM Community Earth System Model	16
CMIP Coupled Model Intercomparison Project	5
CH₄ methane	19
CO carbon monoxide	19
CO₂ carbon dioxide	4
CV cross-validation	30
DECK Diagnostic, Evaluation, and Characterisation of Klima	5
ECS Effective Climate Sensitivity	15
ENSO El Niño-Southern Oscillation	8
ESM Earth System Model	4
ESMValTool Earth System Model Evaluation Tool	1
GHG Greenhouse Gas	4
GPP Gross Primary Productivity	20
GSAT global mean near-surface air temperature	9
GtC gigatonnes of carbon	19
IAM Integrated Assessment Models	7
LongRunMIP Long Run Model Intercomparison Project	17
MDER Multiple Diagnostic Ensemble Regression	31

MIP Model Intercomparison Project	5
ML Machine Learning	2
MMM multi-model mean	23
NAO North Atlantic Oscillation	8
NCAR National Center for Atmospheric Research	16
PDF probability density function	25
ppm parts per million	19
RCP Representative Concentration Pathway	7
RMSE root-mean-square error	29
ScenarioMIP Scenario Model Intercomparison Project	6
SSP Shared Socioeconomic Pathway	6
TCR Transient Climate Response	17
TOA top of the atmosphere	12
WCRP World Climate Research Programme	5
WGCM Working Group on Coupled Modelling	5

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Declaration of Authorship

I assure that this thesis is a result of my personal work and that no other than the indicated aids have been used for its completion. Furthermore I assure that all quotations and statements that have been inferred literally or in a general manner from published or unpublished writings are marked as such. Beyond this I assure that the work has not been used, neither completely nor in parts, to pass any previous examination.

Oberpfaffenhofen, March 2021

Manuel SCHLUND