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Simplifying the cloud microphysics and aerosol representation of a global aerosol climate model

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Abstract

Climate models are large and complex constructs. They are built and used with different purposes in mind, to generate realistic projections or aid in developing understanding. A common approach to model building is to try to represent all processes that are deemed important for a specific climate system compartment. Aerosols and cloud microphysics are two features of the climate system that influence the radiation balance as well as the hydrological cycle. Since the associated processes cannot be resolved explicitly on the coarse climate model grid, their effect on grid-scale variables needs to be parameterized. In developing such parameterizations, it is often assumed that greater detail is beneficial since it increases the representativeness of the model compared to the physical world. Thus, model complexity has become a norm in climate model development.

However, model complexity also has negative effects. Among others, it hinders understanding and the interpretability of the model. Here I address model complexity by simplifying the aerosol and cloud microphysics scheme of the global climate model ECHAM-HAM.

First I developed a method to assess the potential for simplifications in the cloud microphysics (CMPs) scheme. I implemented parameters for perturbing a processes' effect on model variables. Simulating many simultaneous perturbations I generated a perturbed parameter ensemble (PPE). Constructing a surrogate model from the PPE allows us to apply a quantitative sensitivity analysis. Indeed, I find that model sensitivities are dominated by one of the four investigated cloud microphysical processes, while two are negligible in comparison and thus could be simplified.

I go on to apply this methodology to the whole two moment (2M) CMPs scheme of the aerosol climate model ECHAM-HAM. Perturbing 15 processes, I find that 8 have potential for simplification. Indeed, setting processes' effects constant or to a prescribed climatology or even removing some gives satisfying results for 7 of them. Importantly, the derived simplifications are robust in different climate states, preserving the models' fit for climate projection applications. Repeating the same analysis for the alternative P3 scheme, I see shared sensitivities. However, the process of ice crystal autoconversion, which dominates sensitivities in the 2M scheme is unnecessary in the P3 scheme and thus the latter scheme exhibits more balanced sensitivities.

Third, I turned to the aerosols which impact clouds via their role as nucleation centers for cloud droplets or ice crystals. Since our scientific interest focuses on the CMPs, I attempted to drastically simplify the aerosol module. I developed two simplifications in the form of prescribed climatologies, one for potential cloud condensation nuclei (CCN) and one for aerosol mass and number concentrations. In terms of global cloud variables, the climatological approach proves promising. However, a mean climatology of CCN underestimates cloud droplet number concentrations in the Southern Ocean. This bias can be eliminated by incorporating a treatment of hygroscopic growth in the climatology. At the same time, the climatological treatment enables large computational savings.

The sensitivity analysis and simplifications highlight scheme redundancies and peculiar model behaviour. Thereby the method of simplification is shown to generate new understanding, enable a new perspective, and open up promising avenues for model development. The results of this work call into question the complexity paradigm in climate modeling.

Zusammenfassung

Klimamodelle sind große und komplexe Konstrukte. Sie werden für unterschiedliche Zwecke entwickelt und genutzt, um realistische Projektionen zu generieren oder um zu einem besseren Verständnis beizutragen. Ein verbreiteter Ansatz in der Modellentwicklung ist der Versuch einer Abbildung aller Prozesse, die für eine spezifische Klimasystemkomponente Relevanz zu haben scheinen. Aerosolpartikel und die Wolkenmikrophysik sind zwei Teile des Klimasystems, die sowohl die Strahlungsbilanz als auch den hydrologischen Kreislauf beeinflussen. Weil die damit verbundenen Prozesse auf dem groben numerischen Klimamodellgitter nicht aufgelöst werden können, wird ihr Effekt mit Hilfe gitterskaliger Variablen parameterisiert. Bei der Entwicklung solcher Parameterisierungen wird meist angenommen, dass die Berücksichtigung von mehr Details die Aussagekraft des Modells in Bezug auf die Realität verbessert.

Aber Modellkomplexität birgt auch negative Effekte. Unter anderem erschwert sie das Verständnis des Modells und die Interpretation seiner Ergebnisse. In der vorliegenden Arbeit befasse ich mich mit dieser Modellkomplexität, indem ich die Aerosol- und Wolkenmikrophysikschemata des globalen Klimamodells ECHAM-HAM vereinfache.

Zunächst entwickelte ich eine Methode, um Potential für Vereinfachungen im Wolkenmikrophysik (WMP) Schema zu identifizieren. Dafür implementierte ich Parameter, mit denen der Effekt eines Prozesses auf die Modellvariablen perturbiert, also kontrolliert gestört, werden kann. Mit vielen gleichzeitigen Perturbationen generierte ich ein sogenanntes Perturbed Parameter Ensemble (PPE, sinngemäß ein Ensemble von perturbierten Parametern). Ausgehend von dem PPE konstruierte ich ein Stellvertretermodell, um darauf quantitative Sensitivitätsanalyse anzuwenden. Tatsächlich zeigt die Analyse, dass die Modellsensitivitäten von einem von vier untersuchten WMP Prozessen dominiert werden. Zwei der Prozesse sind im Vergleich vernachlässigbar und könnten vereinfacht werden.

Weiter wendete ich die entwickelte Methodik auf das gesamte zwei Momenten WMP Schema des Aerosol-Klimamodells ECHAM-HAM an. Von 15 perturbierten Prozessen haben 8 Potential für Vereinfachungen. Tatsächlich zeigt das Modell geringe Abweichungen in globalen Mittelwerten für Vereinfachungen von sieben Prozessen, in denen ihr Effekt entweder konstant, auf eine Klimatologie oder sogar eliminiert wird. Weil diese Vereinfachungen in verschiedenen Klimazuständen robust sind, wird der Wert des Modells für Klimaprojektionen erhalten. Die Durchführung derselben Analyse mit dem alternativen P3 WMP Schema zeigt geteilte Sensitivitäten. Allerdings ist der Prozess der Eiskristallautokonversion, der im 2M Schema die Sensitivität dominiert, im P3 Schema obsolet. Deshalb sind die Sensitivitäten im P3 Schema ausgeglichener.

Zuletzt wendete ich mich den Aerosolpartikeln zu, die in ihrer Rolle als Nukleationszentren für Wolkentröpfchen oder Eiskristalle die Wolkenbildung beeinflussen. Weil sich unser wissenschaftliches Interesse auf die WMP fokussiert, vereinfachte ich das Aerosolmodul drastisch. Ich entwickele zwei Vereinfachungen in Form von Klimatologien, eine für potentielle Wolkenkondensationskeime und eine für die Massen- und Anzahlkonzentrationen der Aerosolpartikel. Im Hinblick auf global gemittelte Wolkeneigenschaften ist der klimatologische Ansatz vielversprechend und ermöglicht zugleich Rechenzeiteinsparungen. Allerdings unterschätzt eine Mittelwertklimatologie von Wolkenkondensationskeimen die Anzahl der Wolkentröpfchen im südlichen Ozean. Um diesen Bias zu eliminieren, muss die Klimatologie den Effekt des hygroskopischen Wachstums an der Wolkenbasis mit einbeziehen.

Die Sensitivitätsanalyse und die Vereinfachungen offenbaren Redundanzen in den untersuchten Schemata und eigenartiges Modellverhalten. Diese Arbeit zeigt, dass die Methode der Vereinfachung neues Verständnis generieren kann, eine neue Perspektive ermöglicht und neue Wege für die Modellentwicklung eröffnet. Die Ergebnisse stellen das Komplexitätsparadigma der Klimamodellierung infrage.

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Contents

1

Introduction and background

Climate models are huge constructs containing multiple compartments, from the atmosphere to the soil, and a host of processes, from the growth of aerosol particles to sedimenting precipitation particles. They emerge from decades of development, millions of lines of source code and can produce terabytes of data. Climate models' complexity is one of their deeply engrained characteristics. This thesis sets out to question this complexity and how it arose.

1.1 What is a global climate model?

By global climate model (GCM) we mean a model of the atmosphere and other components in the climate system (such as the ocean or land surface) that is implemented into computer code. It aims to include parts of the climate system that are thought to matter for the study of climate, to help researchers generating understanding and to facilitate projections of climate change. In a research context, the models are used and manipulated daily. Their results, downsized to a few central numbers, also are a central pillar of climate change assessments and projections and thus influence policy making. For example, the IPCC bases its assessments largely on such GCMs, in combination with observations and expert judgement.

1.1.1 Why do scientists construct models?

Before delving into the specifics of climate modeling, it is illustrative to ask why scientists construct (computer) models in the first place[1,2]:

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[1] I recognize there is a host of work on the differences of models and experimentation or observations as scientific tools, and the specifics of computer models from a philosophy of science perspective, but leave out its discussion here and refer the reader to e.g. Humphreys (2004), Winsberg (2006), Humphreys (2009), Parker (2021), and Parker (2022b)

[2] Note that this non-exhaustive list of reasons to model the climate system is closely related to the modeling visions discussed in 1.3.2.

- **System complexity** – Natural systems involve so many components, processes and interactions that they do not fit into a single human's understanding. Computer models and their simulations can help us make sense of these natural systems and their dynamics (Gramelsberger et al., 2020).

- **Mediating models** – In trying to represent these natural systems, models "aim to encapsulate our understanding of the system" (Hrachowitz and Clark, 2017). Modelers translate our theories about a system into computer code. Fittingly, Winsberg (1999) has thus described models as "rich physical constructs that mediate between our theories and the world." Accordingly, environmental models can be characterized as mediating models (Morrison and Morgan, 1999; Babel and Karssenberg, 2013[3]).

- **Numerical solving** – When the system to be described by the model is large and complex, the equations describing the system may not be solvable analytically (as is the case for the Navier-Stokes equations describing atmospheric motion that are at the base of the dynamical core of every atmospheric model). Then numerical approximations become the only way to solve and evaluate these equations, and computers help to automate the task.

- **Experimental tools** – Standing in for the natural system under study, models allow for investigation of and experimentation with the system that would not be feasible or desirable to conduct in reality (Lahsen, 2005). Modeling can thus also be regarded as a tool for asking "What if?".

- **Communication objects** – In pouring theories or knowledge into model code, modelers commit to one way they assume the world works. They translate their knowledge and assumptions into the language of math and computer code, which forces them to become explicit. Thus models can serve as communication objects, embodying a "collection of testable hypotheses" (Crout et al., 2014, citing Jameson et al. (1998b)) and data in a readable and comparable way (Randall and Wielicki, 1997).

- **Book-keeping** – At the extreme, climate models can be seen as a "space in which all scientific knowledge about processes relevant to climate needs to be represented and synthesized" (Heymann and Achermann, 2018). The climate science community can hence be characterized to use models as "book-keepers"[4].

In summary, scientists use climate models to construct a "world in a box" (Miller (2004), citing Edwards (2001)). They serve to organize knowledge and understand complex systems (Hulme, 2013).

[3]Babel and Karssenberg (2013) summarize this view for hydrological modeling. Throughout this chapter I refer to hydrology papers often as this community is further advanced in certain reflective modeling discussions, and I assume that key reflections about numerical models apply to different climate science disciplines.

[4]Wendy Parker used this term in a discussion we had in March 2022. This modeling motivation can culminate in the "mirror view" that aims to mirror the real system observations with the model (Parker, 2022a) and closely links to the representative vision of modeling described in Sec. 1.3.2.

Box 1: "Models are imperfect"

> *...so the key to success is how we deal with these imperfections*
>
> — Stensrud (2007)

For the work presented in the following, it is important to realize that numerical models such as GCMs are naturally "wrong". Knutti (2008) states that "all current climate models are known to be empirically inadequate", referring to their inability to match observations (citing Sanderson et al. (2008) as an example). In fact, as Oreskes et al. (1994) argue, "verification and validation of numerical models of natural systems is impossible." It is thus not even clear how a model could be (proven to be) "correct". What one can argue for instead, when justifying model use for a scientific question, is the adequacy-for-purpose of the model at hand (Parker, 2009). There is no clear scientific rule for the design of a model, but modeling is based on knowledge, plausibility, pragmatic considerations and restrictions by computer power (Heymann, 2010a). Usually only one out of a range of alternative model formulations is chosen (Crout et al., 2009; Hourdin et al., 2017). As Sundberg (2009) states, "there is no algorithm for reading of models from theories. Therefore, theories function as constraints and not as determinants in the process of simulation and construction." In addition, numerical climate models contain parameters that are known to be artificial and necessarily incorrect (see the discussion of the autoconversion scaling factor in Sec. 2.3.3 and Sec. 3.3.1). Thus, Bjorn Stevens has called climate models "fantasies" (Stevens, 26.09.22)[a]. However, while highlighting this limitation of GCMs is important, it is not meant to criticize their value. Instead, it serves to view GCMs as "valuable, yet flawed, tools" (Stensrud, 2007, pg.394). In appreciation of the difficulty of constructing a GCM, it is remarkable that numerical predictions have value (Stensrud, 2007).

[a]While he recognizes that this naming is provocative to the public and scientists who communicate with the public, he claims that honesty in this regard is important.

Box 2: Models are social constructs

There is no Archimedean point outside the world upon which to stand. One is always inside the world, and the world is messy.

— Schaffer (2015)

Talking about numerical models, one tends to forget that these are not pure physics and equations, but that they consist of files that are written by humans (Menard et al., 2021). Melsen et al. (2018b) call this the "naturalizing force" of modeling, which makes it appear "as if these human-invented models would represent 'nature'." They claim that this "often conceal[s] the model's social and political construction" and hides underlying assumptions and conventions.

In model construction, modelers have to make "literally thousands" of "unforced" methodological choices (where one option is not "objectively better" than the alternatives) (Ward (2021) quoting Winsberg (2012)). The opacity of complex models[a] further allows such manipulations to be implemented without deeper theoretical justification (Heymann (2010a)). In these decisions, epistemic and non-epistemic considerations play a role, including simply pragmatic ones. Thus "a model is shaped by the group that constructs and modifies it" (Dalmedico, 2007). Hence, even when modelers are seen to simply translate climate knowledge into code, models are not neutral, as "knowledge of climate always carries with it beliefs and values about the world it is seeking to describe" (Mahony and Hulme, 2018). Physicists constructing climate models bring a particular set of values and are part of a scientific culture (Heymann and Dahan Dalmedico, 2019)[b]. Modelers' values have been shown to influence model construction and results[c]. Hence, we can conclude that "models are social constructs, making model results time and place dependent" (Melsen, 2022).

[a]meaning that the relationship between inputs and outputs is not open for inspection

[b]Modelers of a specific discipline form "epistemic communities of like-minded scholars" (Melsen et al., 2018b), whose emergence is detailed in Sec. 1.2.3.

[c]for climate science and modeling see Mayer et al. (2017), Parker and Winsberg (2018), Pulkkinen et al. (2022), and Undorf et al. (2022); for hydrology see e.g. Deitrick et al. (2021)

1.1.2 Parameterizations

At the core of atmospheric models are dynamic equations. Since we have no analytical solution for those, they need to be solved numerically and hence discretized to the grid of the model. This approach has been a huge success for numerical weather prediction and the start of the atmospheric modeling enterprise (see Fig. 1.2). However, there are many other processes that cannot be resolved explicitly in atmospheric models. For example, a single plant's growth process or the formation of a cloud occur at scales much smaller than the model resolution ($1.875° \times 1.875°$ in the case of our GCM ECHAM-HAM). Hence, to include them in models, these processes need to be represented in terms of their effect on grid-scale variables, such as land surface albedo or relative humidity, meaning that the processes' "climatic effect is estimated rather than actually calculated" (Dalmedico, 2007). Such a representation of unresolved processes is termed a parameterization (Stensrud, 2007; Sundberg, 2007). The approach to develop parameterizations can be distinguished ideal-typically into theoretical and experimental approaches (Sundberg, 2007), starting either from physical laws or observational data. In practice, global climate model resolution is so coarse that it renders purely theory based parameterizations impossible. Thus parameterizations always include certain empirical elements.

In principle, moving to higher model resolution allows to represent processes physically resolved rather than parameterized and thus high hopes are put into the move to global high-resolution models (Marotzke et al., 2017). While this hope is justified for some processes such as convection, the need for other processes' parameterization (such as for cloud microphysics) will remain, at any conceivable resolution (Stensrud, 2007, pg. 6). There are always processes that occur on scales smaller than the model resolution, and hence nearly all models[5] incorporate parameterizations (Parker, 2003).

In developing parameterizations, the discussion on model development being non-deterministic (see Box 1) becomes especially urgent. In fact, for parameterizations, "scale-dependence and some degree of arbitrariness is the rule rather than the exception" (Shackley et al., 1998). This is because in parameterizations, per definition, processes are not being represented explicitly but approximated[6]. This leaves room for epistemic and pragmatic values to enter model development, such as completeness, realism, complexity, simplicity, computational stability and efficiency (Undorf et al. (2022); see Box 2). Sundberg (2009) has interviewed modelers on parameterizations and one of the interviewees stated that "It's a bit arbitrary how to do parameterizations. Different researchers can have very different opinions about what they think is the best and it is hard to say who's wrong, but everybody is right in some way" (quote from interview 7). Because parameterizations include interactions but are only approximations, one even has to be "very careful when you

[5] Note that there are other proposed approaches to model climate than the reductionist approach that requires parameterizations. For example, Lovejoy (2022) has argued for the development of stochastic macroweather models that exploit behaviour on scales larger than the weather scale and weather prediction limit without explicitly representing features smaller than this scale.

[6] One might object here that there exist effective models of small scale processes such as diffusion or the Navier-Stokes equations. If one could get such physical laws for the behaviour of cloud particles at km scales, one might get a non-approximate parameterization. However, this debate seems rather philosophically out of scope as it is tangled up in what one might call truth in science (Kuhn, 1996) and where approximations start. Practically, in climate science the Navier-Stokes equations are termed rather physical laws than a parameterization.

have parameterizations in a model so that you don't parameterize the same thing several times" (quote from interview 15). The interviewee continues: "I think that is why you go to the mathematical and physical laws and parameterize the processes [from them]." (Sundberg, 2009, Interview 15), demonstrating the thought process from realizing model weaknesses to calling for more physics as a cure that I discuss next.

Role of physics Due to the ambiguity in creating parameterizations, there are conflicting views in the research community regarding what makes a good parameterization. Physical background of a parameterization (or model) is often invoked as a justifying strength. In light of the fact that models cannot be validated (Oreskes et al., 1994) and that empirical parameterizations impair the representational accuracy of a model (Knüsel and Baumberger, 2020), the "physical" basis of a parameterization serves as an anchor and a promise of correctness (Knutti, 2008; Hrachowitz and Clark, 2017). For example, it is often argued that to be able to extrapolate model simulations into different climate states, parameterizations "need to be based on (or at least loosely inspired by) physical, chemical or biological principles" (Baumberger et al., 2017). By basing parameterizations on physical theory or observations, model developers try to come close to a theoretically justified representation. Consequently, experimentalists focus on detailed studies of physical processes to then derive parameterizations for a model (e.g. Vergara-Temprado et al. (2017) and Lohmann et al. (2020))[7].

However, the role of physics in models is also questioned[8]. One can argue that on climate model grid scales parameterizations are not (and cannot be) a realistic representation (Heymann, 2020) and that therefore processes represented in models are not meant to be interpreted physically (see e.g. Melsen and Guse (2019, pg. 10545)). To put it simply but provocatively, "the model doesn't care what the process is called" (Ulrike Lohmann, personal communication). Whether a process that combines two liquid hydrometeors into one large one is called cloud droplet autoconversion or collision-coalescence does not matter to the model per se, but of course the formulations of the process representations will differ. In contrast, what is meant by processes or variables in one model may differ so widely from their meaning in another model that it makes their physical basis questionable (Dalmedico (2007), referring to Herve Douville).

In that sense, no one would argue that the model is piecewise "correct" or that parameterizations are (the degree of wrongness is of course dependent on the process). In addition, even if there were such a thing as a physically correct parameterization, it would likely not lead to the best model performance because it may disturb the models' "balance of approximations" (Lambert and Boer, 2001; Parker, 2009) [9]. Thus, there is no direct link from physics to a good parameterization. Despite or

[7]Whether this is the most promising route for model development is questionable. Modelers such as Jakob (2010) criticize that process studies aimed at model improvements do not address major model shortcomings. They see the need to "establish a solid connection of process-oriented model development to overall model errors".

[8]Here, the issues in parameterizations already bring out the contrast between different model views (Dalmedico, 2007), namely between understanding and realistic representation, corresponding to the heuristic and representative vision, that will be discussed further in Sec. 1.3.2

[9]However, in the heuristic and representative vision (see Sec. 1.3.2), constraining a process physically means less degrees of freedom in the model and thus is clearly an advancement.

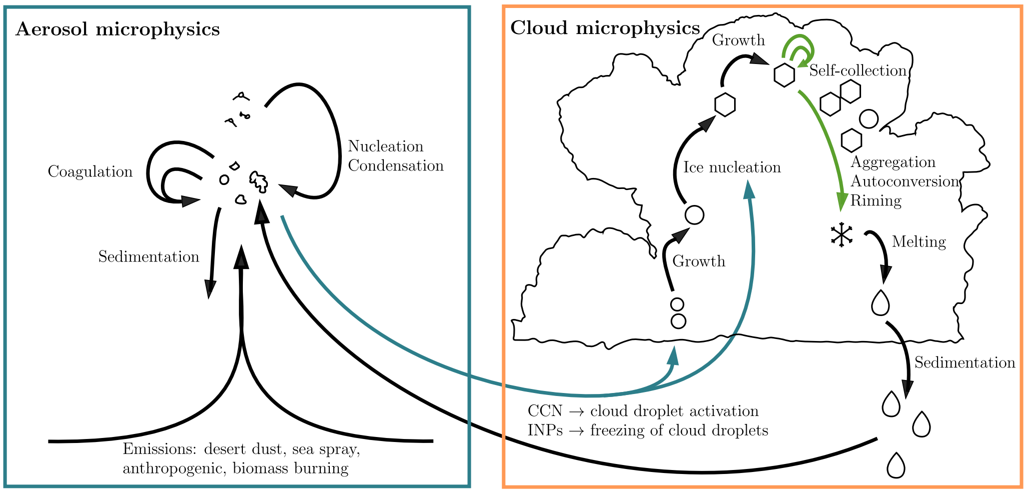

Figure 1.1: Schematic depiction of aerosol and cloud microphysics that are represented in our GCM ECHAM-HAM and the object of this work's studies (right side inspired by Lohmann et al. (2016, Fig. 8.19)). Chapter 2 tests the simplification potential of four cloud microphysical processes (highlighted in green). Chapter 3 expands this investigation to all cloud microphysical processes in two different cloud microphysics (CMPs) schemes (highlighted in orange). Chapter 4 studies the link between aerosol and CMPs, which is the activation of cloud droplets on aerosols acting as cloud condensation nuclei (CCN) or ice nucleating particles (INPs) and aims to simplify the whole aerosol module HAM by replacing it with a climatology (highlighted in blue). For more details on the processes see the respective Chapters and especially Figures 2.1, 3.2, 3.3, and 4.2.

even because of this ambiguity and the fact that parameterization development offers no easy answers, it is a challenging area of research.

1.1.3 Aerosols and cloud microphysics

One particular component of global climate models that this work is focused on are aerosols and cloud microphysics (see Fig. 1.1). They exert a significant influence on the radiative balance and hydrological cycle of the climate system. Next to direct radiative effects, aerosols act as cloud condensation nuclei (CCN) or ice-nucleating particles (INPs). They thereby influence cloud formation and cloud phase, which in turn influences the cloud's radiative impact (Tan et al., 2016; Matus and L'Ecuyer, 2017; Lohmann and Neubauer, 2018). In a cloud hydrometeors interact with each other and with the environmental conditions. These cloud microphysical processes modulate the aerosol-cloud interactions (ACI, see Lohmann and Feichter (2005), Lohmann (2017)) and exert an influence on clouds and climate themselves (Undorf et al., 2022). However, our understanding of ACI is incomplete and their quantification uncertain (Boucher et al., 2013; Bellouin et al., 2020). In addition, uncertainties in cloud microphysics (CMPs) propagate to enhance uncertainties in ACI (Gettelman, 2015). CMP effects and ACI are inherently difficult to quantify, because – like an archetype of the parameterization problem – here microscopic particles have global scale climate influences (Korolev et al., 2017; Bender, 2020; Morrison et al., 2020; de Jong et al., 2022). As for other parameterizations, there are numerous approaches on how to parameterize cloud and aerosol microphysics (see e.g. de Jong et al. (2022) for the distinction between bulk and bin schemes). Their treatment has grown increasingly sophisticated, with the motivation to enhance realism and address uncertainty (Burls and Sagoo, 2022), but their sophistication introduces additional uncertain parameters (Sullivan et al., 2022) (see Sec. 1.3). At the same time, results from different schemes differ, even when using the same base model and dynamics (Sullivan et al., 2022). Randall et al. (2003) summarize the state of affairs aptly: "There is little question why the cloud parameterization problem is taking a long time to solve: It is very, very hard."

1.1.4 The global aerosol climate model ECHAM-HAM

The global climate model employed and investigated in the following chapters is ECHAM6.3-HAM2.3 (Neubauer et al. (2019) and Tegen et al. (2019), termed ECHAM-HAM in the following). It consists of the land surface module JSBACH (Reick et al., 2013), climatological ocean surface treatment, the aerosol module HAM (Stier et al., 2005) (for more details see Chapter 4), and an extended cloud microphysics module (which is described in more detail in Chapters 2 and 3). The latter has seen continuous development and sophistication (see Fig. 1.2), from the introduction of prognostic equations for the cloud liquid and ice mass mixing ratios (Lohmann and Roeckner (1996), first moment) to the introduction of prognostic cloud droplet and ice crystal number to account for aerosol effects (Lohmann et al. (1999) and Lohmann (2002), second moment).

1.2 History of climate modeling

> *Reflection is the courage to make the truth of our own presuppositions.*
>
> — Heidegger (1996), The Age of the World Picture

As model development is path dependent and models are social constructs, it is helpful to reflect how they came about and were developed within climate science (see Fig. 1.2) to understand their present condition.

Alexander von Humboldt, a pioneer of scientific climatology, defined climate as "all changes in the atmosphere which noticeably affect the human organs" (Heymann, 2010b). Humboldt was a representative of 19th century climatology (Heymann and Dahan Dalmedico, 2019), when meteorology and climatology were two distinct fields (Heymann, 2010b). In 1904, the meteorologist Vilhelm Bjerknes managed to summarize all meteorological processes in the atmosphere into seven parameters and six differential equations (Heymann, 2010b). Hence the first half of the 20th century saw the emergence of dynamic meteorology, "a reductionist physical science, interested in the mathematical description of meteorological parameters" (Heymann, 2010b). Heymann and Achermann (2018) argue that this physical view manifested in equations came to replace human-oriented climatology with physical reductionism[10]. Equations based on the laws of physics allowed for the possibility of predictions (Heymann, 2010b). In 1922, Lewis Fry Richardson was the first to manually compute a weather prediction, and John von Neumann managed to compute the first

[10]Reductionism refers to the idea that a complex system is made up of smaller entities (see Sec. 1.2.3).

weather prediction based on computer calculations (Heymann, 2010b). When Norman Phillips performed the first long time weather prediction with a model with a simplified version of Bjerknes' equations it was taken as a great success that cyclone patterns evolved "naturally" in the simulations (Heymann, 2010b). From these weather models, climate models emerged, which "initially served heuristic purposes" (Heymann and Hundebol, 2017). Already in the 1950s and 1960s, heuristic modelers followed the research strategy of expanding GCMs with more sub-models (Heymann, 2020).

World War II and the early cold war fueled modeling ambitions. New tools (such as computers) emerged. Authority and resources were granted to science and technology, and expectations placed upon them (Heymann and Dahan Dalmedico, 2019). Erickson et al. (2013) have termed "Cold War rationality" the "deep belief pervading this era that all systems, natural and social, could be understood, modeled, and controlled, provided sufficient resources were made available" (Heymann and Dahan Dalmedico, 2019)[11]. Thus, digital computing was a product of, but also supported the Cold War emphasis on surveillance, planning, prediction and control (Heymann et al., 2017b, pg. 34).

The societal perception shifted in the second half of the 20th century when overwhelming technological power raised fears of a loss of control (Heymann, 2010b). In the 1970s, "enthusiasm for environmental control had faded" and gave place to environmental concern, but "confidence in numerical approaches" persisted (Heymann, 2020). This environmental paradigm brought the focus of climate science on predictive modeling (Heymann, 2020). In the 1970s, a culture of climate projection emerged and resources were shifted from developing and testing models to their application (Heymann, 2020). Francis P. Bretherton and Klaus Hasselmann called for a broader modeling program that represented other subsystems of the climate system than just the atmosphere, in an effort to more realistically represent this complex system, and thus conceived the field of Earth System Science (Hasselmann, 1979; Bretherton, 1988; Heymann and Hundebol, 2017; Heymann and Dahan Dalmedico, 2019)[12]. The global view of Earth System science corresponded to globalisation in other realms, such as the emergence of satellites that further enforced the idea of a "global climate" (Heymann, 2010b).

By 1988 the IPCC and with it a scientific culture and identity had emerged, which included climate projection, public communication and deliberate connection of science and politics (Heymann, 2020). The cornerstones of climate research have moved far from the classical climatology of Humboldt's days (Heymann, 2010b): we are more interested in the human impact on climate than in the effects of climate on humans, climate has become a global phenomenon that is perceived not as stable but as changing in time and which we aim to model with global models that aim for a grasp of the complex global climate system.

[11] This belief in the power of ever increasing resources is still manifested in the present great push for ever higher resolution weather and climate models (Palmer, 2014; Palmer and Stevens, 2019; Schär et al., 2020; Hewitt et al., 2022).

[12] Which still today demands a global, holistic view of the climate system and connects this to policy aspirations, as e.g. Rauser et al. (2017) claim that a "coordinated, interdisciplinary, and truly global approach to Earth system science is the best means to foster understanding of the complex interplay of Earth's processes and to develop applicable tools to confront the challenges facing society both now and in the future."

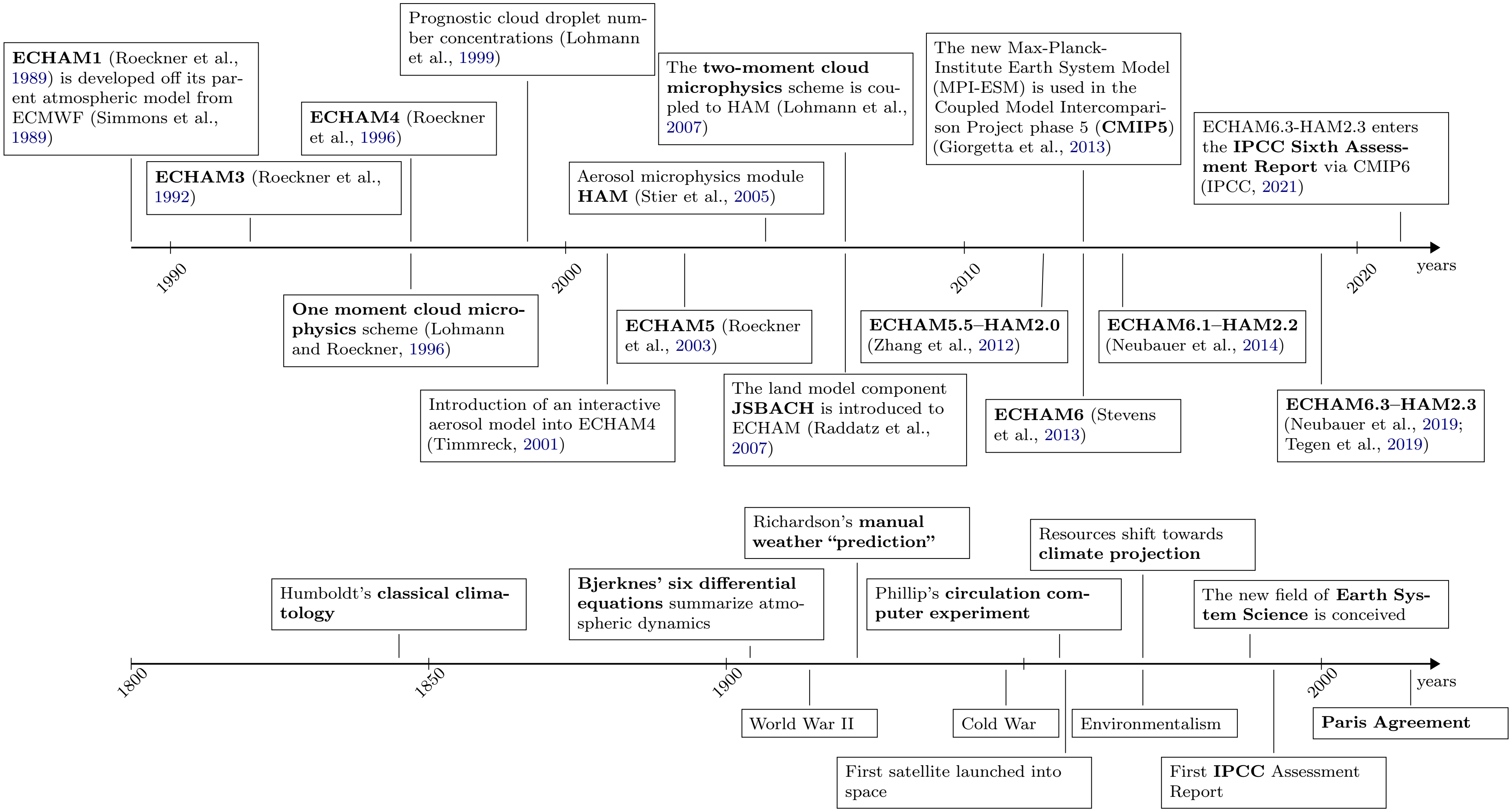

Figure 1.2: Timeline of **a)** ECHAM-HAM development and **b)** climate modeling and societal history, compiled from the sources mentioned in Sec. 1.2, CarbonBrief (2018), and additional literature search. Note that the development of ECHAM-HAM may also be interestingly put into perspective with its positioning in the model family tree or genealogy (Pennell and Reichler, 2011; Knutti et al., 2013; Kuma et al., 2022).

1.2.1 Co-production

In its evolution, climate science and in particular climate modeling interacted with society (as has become apparent in Sec. 1.2 and Fig. 1.2). "Co-production" terms the idea that science and societal orders are being produced together (Jasanoff, 2010; Heymann and Dahan Dalmedico, 2019).

On the one hand, climate science and modeling is co-produced with climate politics (Shackley and Wynne (1995); see Fig. 1.3). Climate policy signals to GCM development that climate change simulations are needed, while GCMs signal to policy that climate change projections are 'do-able' and that climate change is a serious issue, which grants climate policy legitimacy (Shackley et al., 1998; Shackley et al., 1999). Thus GCMs have become a "common currency" between scientists and policy makers, where each gains in intellectual, scientific, and social terms (Shackley et al., 1998). In particular, the IPCC reinforced a global, systemic understanding of climate and climate change, but also the necessity for and the possibility of a global politics of climate (Miller, 2004). Modeling centers are compelled to use GCMs for projections, for funding obligations, or because of pressure from funding agencies and government departments, or desired public status and relevance (Shackley et al., 1999; Heymann, 2020).

On the other hand, climate modeling is co-produced with other scientific domains. GCM science and development signal to surrounding sciences that specialist knowledge is needed at sub-grid scales, while the surrounding sciences reinforce the notion that model evaluation and extension is 'do-able' and desirable (Shackley et al., 1998). Thus, Heymann (2013) argues that models and trust in models were co-produced. Shackley et al. (1998) highlight that other disciplines produced trusts in GCMs as well, because "by perceiving the advantages and opportunities of collaboration with GCMers [...], these other [...] scientists are effectively endorsing and advocating GCMs". Indeed, model simulations may serve to illustrate the impact of one's work. Also experimentalists justify their research with the need for improved GCMs (Shackley et al., 1998; Sundberg, 2009). Similarly, GCMs were developed in co-production with the climate impacts and policy community. The latter two signal that climate projections are desirable, while GCM developers signal that these projections are 'do-able' and highlight climate change as a global problem. Thus, Shackley et al. (1998) argue that GCMs are supported in part because they help to create an interactive and international community of scientists and policymakers[13].

Lastly, models and the model development or user teams co-produce. A research team develops a model, but also "a research team is built around its investigation of a model and its understanding of a model's particular characteristics"(Dalmedico, 2007). This co-production is illustrated by the finding from Addor and Melsen (2019) that "hydrologists tend to stick to the model they have experience with, and rarely switch to competing models, although these models might be more adequate given the study objects".

[13]Note that Henderson-Sellers and McGuffie (1999) answered Shackley et al. (1998) disagreeingly. I read their response not as disagreeing with the points that I mention above, but rather pointing out that modelers are not naively subjected to these forces but aware of them.

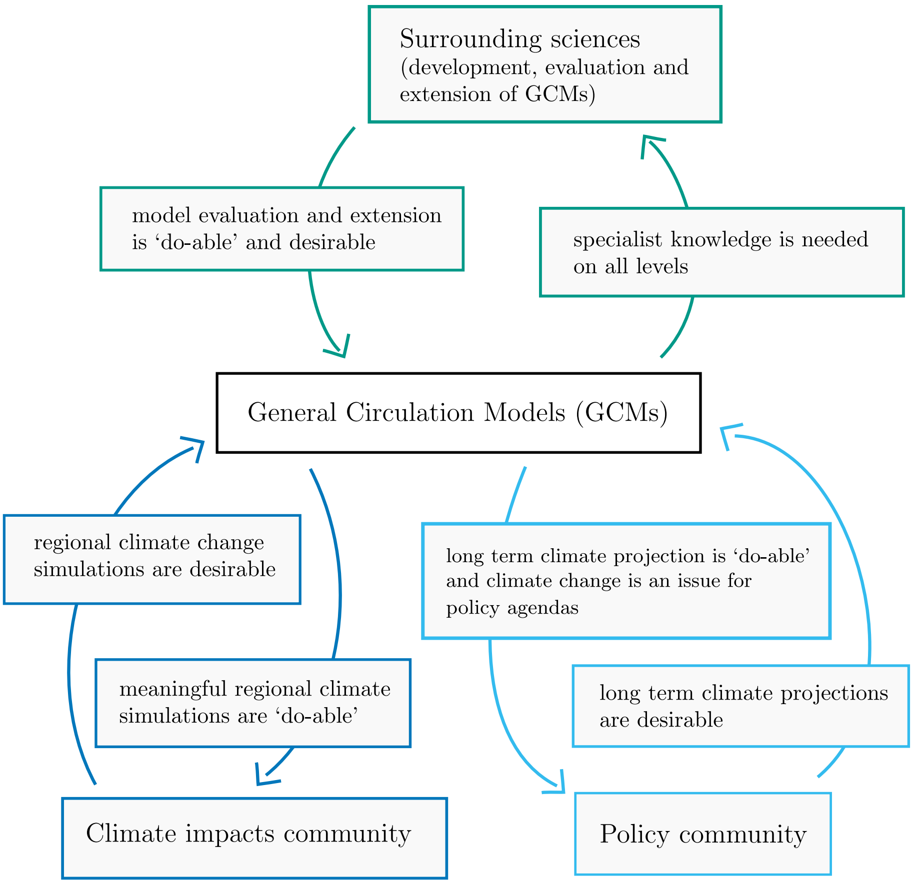

Figure 1.3: Illustration of the co-production of climate modeling between model developers, climate policy, surrounding sciences and the climate impacts community (adapted from Shackley, Simon, Peter Young, Stuart Parkinson, and Brian Wynne. “Uncertainty, Complexity and Concepts of Good Science in Climate Change Modelling: Are GCMs the Best Tools?” Climatic Change 38, no. 2 (1998): 159–205. https://doi.org/10.1023/A:1005310109968).

Box 3: Models have power

> *Modeling and simulation have transformed the toolbox of exercising power and shaping the world. The promises of modeling [. . .] have been sources of epistemic and political power, fundamentally re-shaping expectations about the links between nature and society, science and politics, and technology and culture.*
>
> — Heymann et al. (2017b)

Working with climate models as in this thesis, it is important to reflect upon the fact that these models exercise power. Their ability to become surrogates for reality, their integrative capacity and their unique position as tools to understand the influence of humans on the climate system, have given them a "hegemonic status" (Rödder et al., 2020). The global view of such models and Earth System Science in general enables a new kind of governmentality (Lövbrand et al., 2009) and new forms of authority. As Melsen et al. (2018a) conclude, "models are 'social and political actors' in and by themselves". They act and exercise power in multiple ways:

Future making – Historically, the notion of futures is young. Only being able to conceive futures that could be influenced by human forces allowed for the idea of simulating the future (Heymann et al., 2017a, Intro). In climate simulations, modelers engage in the "generation of possible or desirable climate futures" (Heymann and Dahan Dalmedico, 2019; Rödder et al., 2020). Seeing the influence of the sciences on the climate discourse, Hulme (2008) therefore provocatively asks "Who speaks for the twenty-second century?".

"World building" (Edwards, 2001) – Climate models reproduce a certain understanding and vision of the world (Heymann and Dahan Dalmedico, 2019), while they are at the same time seen as to resemble truth (Boelens, 2015). Thus they influence what is possible to look at, how we can imagine to intervene in the system, and also which ideas or understandings we cannot develop because they are outside of the model world (Heymann et al., 2017b; Heymann and Dahan Dalmedico, 2019).

Global view – As discussed above, global climate models have co-produced with globalist politics and imaginations, portraying and producing climate knowledge "with bird-eye view from above" (Heymann, 2019; Mahony and Hulme, 2018). This globalization of climate change influences the conceivable and agreeable space of solution or counter measures (Heymann et al. (2017b, pg. 35), citing Miller (2004) and Lövbrand et al. (2009); Mahony and Hulme (2018)).

Authority – Sophisticated models and the quantitative results they produce carry authority (Heymann et al., 2017a; Heymann et al., 2017b; Heymann, 2019), not only for themselves but also for the human actors involved. Heymann et al. (2017b, pg. 35) attest that "on the level of states, the authority to make legitimate contributions to climate knowledge and discourse [. . .] seems to require the operation of a national climate modeling [. . .] effort". This authority is reinforced by the use of advanced technology and maintained by large-scale infrastructures and powerful institutions (Heymann, 2019). This authority has lead other scientists to motivate their research with climate modeling progress (Shackley et al., 1998; Sundberg, 2007) and influences science funding.

1.2.2 Interaction with climate change

Climate knowledge based on GCMs occupies a strong position, with a large social, media and political impact (Heymann, 2020). Sundberg (2007) even claims that "climate models have become gatekeepers for claims about climate change" (Sundberg, 2007). The role of GCMs for investigating the threat of climate change and for raising it as a serious issue on the political agenda cannot be overstated (Shackley et al., 1998; Heymann, 2013). Methodologically, they allow for attribution as well as process and sensitivity studies and have thus contributed heavily to our understanding of the climate system and climate change (Edwards, 2001; Parker, 2003). Moreover, for climate change mitigation efforts, models serve to evaluate the effects of different policy options (Edwards, 2001).

However, in the process GCMs sidelines alternative approaches to understanding climate (Heymann et al., 2017b, pg. 25)[14]. Hulme (2008) goes so far as to say that the IPCC "almost trade-marked Climate Change™". At the very least, climate change knowledge and discussions have remained firmly in the hands of natural sciences, circling around projections and a problem-solution or managerial policy framing (Shackley et al., 1998; Hulme, 2008; Mahony and Hulme, 2016). Sarewitz (2004) attests the problem of politics and climate change becoming "scientized" and depoliticized (see also Heymann et al. (2017a), Melsen et al. (2018b), and Rödder et al. (2020)). Rödder et al. (2020) suggest that there is a lack of progress in climate policy "because science has taken center stage but is unable to offer political solutions" (Rödder et al. (2020) citing Grundmann (2018)). As Sarewitz (2004) argues, in fact more science may not solve environmental controversies but make them worse[15]. In fact, the global view of GCMs is separated from local, personal experience and perception (Mahony and Hulme, 2018) and thus opens up a schism of reality (Hulme, 2008; Heymann and Dahan Dalmedico, 2019). Heymann (2019) see this "dehumanization" of the climate concept as a "crucial dilemma behind the

[14] Heymann et al. (2017b) and Heymann et al. (2017a) list as alternative approaches those that emphasize local ecologies and climate-society interactions, indigenous knowledge and humanities, extremes rather than global means, and risk management frameworks for dealing with climate change.

[15] He argues that by scientizing a given political issue, the underlying conflict of values or interests is ignored, and thus the conflict cannot be solved. Relatedly, Glavovic et al. (2022) even call for a moratorium on climate science. Other than Sarewitz (2004) they diagnose the reason for lack of climate action despite of amounting climate change evidence as the broken "science-policy contract". Thus they see no hope of more climate science leading to more climate action.

failure of climate politics".

1.2.3 A scientific culture emerges

Out of historical development and co-production a scientific culture of climate modeling was formed. The scientific culture of climate modelers determines practices, shared values, norms and views of the world (Heymann and Dahan Dalmedico, 2019). Heymann (2020) uses the concept of "codes" to describe the culture of climate modeling. He takes "codes" as a broad term for "foundational interests, concepts, language, practices, approaches, values, standards and rules". He identifies codes of the climate modeling community to be theory-based mathematical modeling, grid-based numerical approximation, radical reductionism, heuristic modeling, model experimentation and validation, parameterization and model expansion. I would argue for another code, namely that climate modeling welcomes and seeks a diversity of models, which distinguishes it from other scientific disciplines (see Parker (2006), Knutti et al. (2010), and Babel (2019) and Horton et al. (2022) and Heymann (2010a) for streamflow and atmospheric chemistry models). We have seen how theory-based mathematical and heuristic modeling have shaped the field historically (Sec. 1.2) and how parameterizations (Sec. 1.1.2) are key to model expansion. For the following discussion, the norms of model expansion and reductionism, which leads to increased model complexity, are of particular interest. Reductionism refers to the idea of reducing a complex system (such as the climate system) to the sum of its parts and interconnections (Shackley et al., 1998; Saltelli et al., 2020a)[16]. While this seems intuitive to atmospheric scientists today, it represented a "significant revolution" (Heymann, 2020). In fact, Shackley et al. (1998) note that "the reductionist argument that large scale behaviour can be represented by the aggregative effects of smaller scale process[es] has never been validated in the context of natural environmental systems". The idea to represent the climate system as the sum of its parts is prone to lead to complexity in formulation. That is because in this reductionist view, more realism requires to represent more system parts in ever more details. For example, increasing the realism of an aerosol module seems to require the addition of different aerosol species and emission mechanisms. Thus, somewhat unintuitively, the code of reductionism has lead to a vast complexity in model formulation.

1.3 Model complexity

As shown in Figure 1.2, historically climate models have included more and more interacting components and added details to those (exemplified by the development of ECHAM-HAM in part Fig. 1.2a, see also Edwards (2011)), which leaves GCMs to be incredibly complex. While model complexity is increasingly recognized and researched, there is a multitude of model complexity definitions, and Baartman et al. (2020) even conclude that "aiming for a single definition of model complexity is neither feasible nor desirable". In this work, what I mean by complexity is the comprehensiveness of the model, the number of processes included, and the number of influential parameters and interactions (Parker, 2003; Crout et al., 2014; Hrachowitz

[16]Heymann (2020) specifically discuss "physical reductionism" and criticizes that representing the climate system by physical equations left human affairs out of the picture.

and Clark, 2017; Puy et al., 2022). Note that when this complexity is excessive and useless, it may instead be called complicatedness (Baartman et al. (2020), referring to Grand (2000)). For climate models the utility of their complexity is unclear a priori and is context dependent. Therefore it cannot be judged excessive and useless a priori, so I stay with the term of complexity.

1.3.1 Why did climate models evolve to become complex?

Arguably the simplest computational models of climate are zero dimensional radiation models. They treat the Earth as a point mass and calculate its radiative equilibrium (Edwards, 2011). Starting from these models, historically it made sense to add more components and processes for the models to be a useful tool to study and predict their behaviour. As models are used to study climate as an interrelated system, naturally their scope grows (Fisher and Koven, 2020).

Thus, more components, processes and detail were added to increase the "descriptive capacity" (Puy et al., 2022) of the model. After all, the Earth system is complex and thus scientists may feel that to represent reality, the complexity needs to be mirrored in the model (Shackley et al., 1998; Fisher and Koven, 2020; Saltelli et al., 2020b). A relation to reality can be argued to be a pre-condition for the usefulness of a model, but can become a primary goal when scientists are improving the realism of their models further and further (Jakob, 2010)[17]. Critics of this approach argue that the addition of details in an attempt to capture reality is merely capitulation in front of a complex system, where scientists cannot think of another way to represent it[18]. Similarly, it may even be argued that humans' psychology tends to favor additive rather than subtractive solutions to a given problem (Adams, 2021).

Knutti (2008) argue that the focus on understanding processes may be a driver behind the wish to reproduce reality accurately in the models. For process studies, the model may even be used for "accounting", collecting the processes that we know of, and assuring us when the processes have a small effect[19]. One may also argue that new knowledge from experiments or theory that is added to a model adds constraints to it. However, often models are detailed where the least is known (Stevens, 26.09.22, personal communication). For example, the effects of aerosol-cloud interactions on climate are repeatedly highlighted as a source of uncertainty in climate change assessments (Boucher et al., 2013; Carslaw et al., 2013; Bender, 2020). At the same time, as shown in Fig. 4.3, the aerosol module makes up about 70% of the computing time of ECHAM-HAM. This contrast may stem from the most active areas of research revolving around uncertain topics, or that scientists focus on their own area of interest and expertise also in developing models (Fisher and Koven, 2020). For land surface models, Fisher and Koven (2020) find that "the historical development pathways by which process complexification has proceeded [...] have been largely ad hoc and based on a collection of institutional, geographic, and individual preferences and interests."

Scientifically, complex models may be used as tools to understand systems and derive simpler process formulations, superparameterizations or to build higher order

[17] Lahsen (2005) even claims that modelers may come to think of their models as reality.

[18] I developed this thought together with Shaun Lovejoy in a discussion in May 2022, who, as mentioned previously, is a proponent of stochastical macroweather modeling.

[19] personal communication Wendy Parker, 14.03.22, see footnote 4

models (Parker (2003, pg. 41), Baartman et al. (2020)). In fact, this is what I attempt in Chapter 4.

Especially in aerosol modeling, it is also often claimed that the addition of processes into the model will help to reduce uncertainties, e.g. in aerosol-cloud interactions (Puy et al., 2022). There may also be pragmatic reasons for the increase in model complexity. For example, Bjorn Stevens has argued that GCM complexity arose in a large part to make the model generally configurable[20].

These accounts from the domain of science itself focus on heuristic and representative reasons, likely inspired by the corresponding modeling visions (see Sec. 1.3.2). History and sociology of science offer different perspectives on how to understand increasing model complexity. Heymann and Dahan Dalmedico (2019) attribute GCMs a holistic aspiration (referring to Heymann and Achermann (2018) and Uhrqvist (2015)). Their aim to represent the Earth system as a whole and to integrate all knowledge unified science. It also gave confidence that GCMs in fact were an adequate representation (see Fig. 1.3; Heymann and Achermann (2018) and Heymann and Dahan Dalmedico (2019)). Complexity and completeness came to be important value terms (Undorf et al., 2022). Comprehensiveness of a model increases trust in the model as well as raises the models' and modelers' authority (see Box 3; Shackley et al. (1998), Dalmedico (2007), Heymann (2010a), Koivisto (2017), and Puy et al. (2022)).

When predictive modeling emerged, this "fueled an expansion of the holistic aspiration" of GCMs, expanding also into economic sciences (Heymann and Dahan Dalmedico, 2019). Models' co-production with politics that drove a desire for more detailed information and especially the IPCC contributed to the development of increasingly sophisticated models (Dalmedico, 2007; Knutti, 2008). The coevolution with technology suggests that the increase in complexity may also be due to "continued availability of ever larger and faster computers" (Stensrud, 2007), as large computing demands make models appear more attractive. Model expansion has become a code of the climate modeling community (Heymann (2020), see 1.2.3) and the complexity of model representation a normative principle (Shackley et al., 1998). Thus, complexity in models has come to be seen as an end in itself (Jakob, 2010; Saltelli et al., 2020b)[21].

While heuristic goals drove the development of the first numerical climate models (Heymann and Hundebol, 2017), the GCMs of today are multi-purpose tools, which are used for projections as well as process studies that aim to derive understanding. In fact, environmental models are used across such a wide range of purposes and scales that they may be called "Model[s] of everything and everywhere", as Addor and Melsen (2019) suggest for the case of hydrology. This "one model to fit all" strategy

[20] Putting it concisely and provocatively, he claimed that the Earth System Model "ICON was developed to be the backend of a domain specific language whose front end was the namelist" (Stevens, 2022), where the namelist is the file where the model user defines the model options for a specific simulation. A domain specific language is a computer language that is geared towards one specific application. Bjorn Stevens thereby refers to the practice of making any doable model configuration easily accessible in the namelist that leads to clutter and misunderstanding of the model itself.

[21] Andrea Saltelli moved from statistically rigorous but purely mathematical sensitivity analysis (Saltelli, 2008a) to publishing calls for more reflections about the blind use of environmental models to inform policy (Saltelli and Piano, 2017). Interestingly, his work appears in both contexts in this thesis.

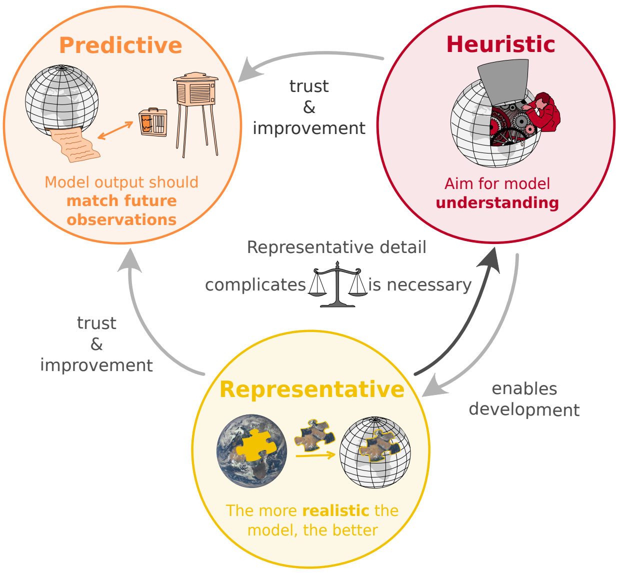

Figure 1.4: Sketch[22] illustrating the different modeling visions and some of their relations. Following one vision may bring progress in another. The conflict between the representative and heuristic vision, that increased representative complexity makes models less interpretable, is what we aim to address in our work of simplification. Note that in the predictive vision, the match of model output to observations may also concern past observations, for example in hindcasts.

(Heymann and Dahan Dalmedico (2019), referring to Uhrqvist (2015)) means that the adequacy-for-purpose (Parker, 2009) of GCMs and hence the appropriateness of details in their formulation is impossible to attest.

1.3.2 Visions

A key to understanding how complexity evolved but also how scientists may judge simplification efforts are the different motivations and cultures that model developers follow or adhere to[23]. These may be conceptualised as epistemic lifestyles, which Shackley (2001) has introduced as a set of intellectual questions, problems, practices, purpose, achievements, ambitions, social networks, connections and necessary activities that form a researcher's character and vision to model development[24]. At least three of these lifestyles or visions can be distinguished (see Fig. 1.4):

- **"Climate model constructors"** (Shackley, 2001) are those researchers that follow the **"representative" vision** (Sundberg, 2009). They aim to represent the climate system in its full complexity, thus for them a more complex model will have a greater truth-content (Shackley et al., 1998). For them, the more

[22]We used various files from wikimedia commons as templates for our sketch reproductions. The files are distributed under a creative commons attribution-share alike license or in public domain. We acknowledge the authors Achodanick, Malchen53, NASA, Mrmw, Ninjastrikers, Agência Brasil, Jahobr and Ibex73.

[23]This discussion is closely linked to Sec. 1.1.1

[24]Melsen (2022) has termed the modeling motivation and philosophy of any given modeler his or her modeling vision. To me, the purist and pragmatic stance of Shackley et al. (1999), the epistemic lifestyles described by Shackley (2001), and the predictive and representative construction of Sundberg (2009) are examples of such modeling visions.

realistic the model, the better. Thus, for a climate model constructor "a single state-of-the-art model exists irrespective of its application" (Shackley, 2001). The ultimate goal would be a model that includes all processes and interactions in a realistic fashion (Schneider and Dickinson, 1974; Shackley et al., 1998; Parker, 2003). Accordingly, for cloud microphysics the dream would be the "numerical representation of all microphysical particles in a single, consistent framework" (de Jong et al., 2022). In designing parameterizations, climate model constructors emphasize theoretical practice and physics (see Sec. 1.1.2, Sundberg (2009)).

- **"Climate seers"** (Shackley, 2001) or **heuristic vision**: in constructing models, they aim for an understanding and exploration of the climate system. Thus, which model is 'state of the art' depends on the question that is being asked. Also, heuristic modelers may pursue modeling purely to advance and help their thoughts[25]. Using e.g. sensitivity analysis, they may use models to corroborate a hypothesis or learn from discrepancies to other models (Oreskes et al., 1994). They may see mathematical models' use in exploring questions, not in asserting answers (Saltelli et al., 2020b).

- **Predictive vision** (Sundberg, 2009): improving the forecast or the performance of the simulation with respect to observational data is the main goal, which leads to choosing practical over the best theoretical solutions.

Of course, the distinction between these lifestyles is not sharp (Heymann and Hundebol, 2017). In practice, many modelers will find themselves sharing thoughts with all of these visions. In fact, choices to be made in model development may often come down to a choice between visions, e.g. asking "What is the goal? [Is it] to have a physically correct parameterization or one that gives a good result?" (Sundberg, 2009). In their most drastic pursuit, visions may even contradict themselves, as e.g. Edward Lorenz has claimed that we cannot gain understanding from a model that achieves representative perfection (Parker, 2003, pg. 75).

Disagreement between model developers can often be traced back to a different weighting of the visions. Similarly, Randall et al. (2003) identify a "deadlock" in cloud parameterization development following the representative vision[26], which they criticize: "We should be asking ourselves: Is it really possible to parameterize all of this complexity with quantitative accuracy?" Koivisto (2017) terms "complexity pitfall" an overemphasis on the representative vision, as he insists that "the main goal of the scientific model is not to be as realistic as possible but to provide better understanding of the studied system.", with this statement being a prime example for the heuristic visions. Also criticizing the representative vision, Carslaw et al. (2017) argue that "the scientist cannot obtain a 'correct' [model] by excessive elaboration" (citing Box (1976)). Held (2005) and Emanuel (2020) criticize the lack of heuristic work where the focus instead lies on model improvements (see also Guillemot (2017), who traces how scientists' visions influence how they develop parameterizations and models). The opposition to different modeling visions may become fierce. For example, Emanuel (2020) stated: "We must resist the wholesale

[25]For example Bjorn Stevens names this as the idea behind his use of modeling (personal communication, 26.09.22).

[26]which of course they don't name as such

migration of atmospheric, oceanic, and climate science away from a traditional curiosity-driven scientific endeavor to the more strictly applied venture of predicting weather and climate."

The differing visions have come in one after the other historically (Heymann, 2020) and now co-exist. As detailed in Sec. 1.2, the first climate modelers were interested in generating physical understanding. Only later numerical prediction was conceived (Heymann and Dahan Dalmedico, 2019), and by the 1970s, model development was pushed to deliver long-term climate projections (Heymann and Hundebol, 2017). Historically, justification of the model has resulted also from successful comparison of the model's results with observations, even if the scientific understanding was insufficient (Heymann, 2010a; Heymann, 2013; Heymann, 2020). Often times scientists have not reflected on their model visions, by themselves or in their working group. They come to adopt their epistemic lifestyle depending on their institution, the relationship of their modeling to the policy making process or how the model's output is used, and their 'style' of modeling (e.g., disciplinary, institutional, or personal career trajectory backgrounds) (Shackley et al., 1999)[27]. Today the same GCMs are used for both projections and heuristic purposes, with representative accuracy being evoked as synonym for truth content. This may lead to problems, e.g. where scientists are using schemes rooted in predictive construction to answer heuristic questions.

1.3.3 Problematic complexity

While increased complexity may be seen as a welcome development, e.g. following the representative vision (see 1.3.2), it brings about a bouquet of problems:

- Model development itself has moved faster than it can be tested. For snow models, Menard et al. (2021) state that "new parameterizations are added faster than old ones are deprecated", which results in a growing user interface and configurations becoming incomprehensible (see footnote 20).

- Complexity likely does not reduce uncertainty (Knutti and Sedláček, 2013; Stevens and Bony, 2013; Carslaw et al., 2018). However, it gives an illusion of certainty, because it makes the uncertainty of results difficult to take into account or even invisible (Heymann, 2013; Bender, 2020; Puy et al., 2022). Puy et al. (2022) put it boldly: "More detailed models may be thought of as more accurate simply because their very design complicates any attempt at proving otherwise."

- The more complex a model, the more free parameters it contains, leaving the model more "wiggle room" (Carslaw et al., 2018). Hulme (2013) have called such models with many degrees of freedom "nervous models". At the same time, the data to meaningfully constrain parameters or processes in environmental models are lacking (Dalmedico, 2007; Hrachowitz and Clark, 2017; Baartman et al., 2020; Puy et al., 2022), but more complex models need more data for the

[27]To be transparent, I want to acknowledge here that I was embedded in the Atmospheric Physics group at IAC, ETH. To me it seems like the group mostly follows the heuristic vision in model construction and use. At the same time, we are well aware that a different configuration of the model is used for climate projections and that the predictive vision seems to be followed in other working groups of our institute.

same justifiability (Guthke, 2017; Burls and Sagoo, 2022). Increasing model complexity also implies that "errors (...) can be much more difficult to find and correct" (Stensrud, 2007).

- The complexity and its authority may hide the effect of ill-constrained minor-looking treatments (Kawai et al., 2022), such as artificial parameters, limits, order, thresholds, parallel or sequential splitting, ordering dependency, timestep or resolution (Kiehl and Williamson, 1991; Teixeira et al., 2007; Donahue and Caldwell, 2018; Barrett et al., 2019; Hieronymus et al., 2022; Kawai et al., 2022; Zarzycki, 2022).
- Similarly, modelers' judgements and choices become hidden in complexity (Shackley et al., 1998) (for subjective decisions in e.g. in hydrological modeling see Melsen et al. (2019) and Mendoza et al. (2016), and Tapiador et al. (2019) for a comprehensive compilation of choices and assumption in modeling cloud microphysics).
- Larger models require more resources to run, which may limit the length, resolution or number of simulations feasible.
- More complex models also require advanced programming skills, and domain scientists may lack the necessary training (Merali, 2010; Barnes and Jones, 2011; Emanuel, 2020).
- Excessive model complexity limits a model's social usefulness and may have "deleterious social-environmental consequences" (Puy et al. (2022), citing (Saltelli et al., 2020b) and Pilkey and Pilkey-Jarvis (2007))

While for Chapter 4 the computing time is a prime motivation, for Chapter 2 and 3 our main motivation lies on the difficulty to understand complex GCMs. Knüsel and Baumberger (2020) have developed a framework for analysing the fitness of a model for understanding a phenomenon. That fitness depends on three dimensions, the representational accuracy, the representational depth or detail of the model, and its graspability (Knüsel and Baumberger, 2020). These dimensions represent a trade off: as accuracy and detail increase, graspability decreases. Thus increased complexity harms the modelers' ability to analyse and grasp model behaviour (Shackley et al., 1998; Fisher and Koven, 2020; Knüsel and Baumberger, 2020). Gramelsberger et al. (2020) call this the "dilemma of growth": "On the one hand, simulation modeling is the method of choice (arguably without alternative) for understanding the dynamics of a system as complex as the Earth System. On the other hand, the growing complexity makes that understanding difficult to achieve." In particular (in addition to the general problems of complexity listed above), there is a specific set of climate model(ing) characteristics, which make a complex model less amendable to interpretation and understanding (see also Knüsel (2020, Sec. 1.2.6.)):

- **Epistemic opacity** names the phenomenon that in complex computer simulations, the relationship between inputs and outputs is 'opaque' and not easily open to inspection or analytical understanding (Humphreys, 2004; Heymann, 2010a; Lenhard and Winsberg, 2010; Heymann, 2013; Rödder et al., 2020). Thus scientists have to devise sophisticated methods to make sense of their models (Gramelsberger et al., 2020), such as process rates diagnostics (Bacer et al., 2021), piggybacking (Sarkadi et al., 2022), pathway analysis (Schutgens and Stier, 2014; Dietlicher et al., 2019), emulation (Rougier et al., 2009; Lee et al., 2011; Holden et al., 2015; Johnson et al., 2018; Tsushima et al., 2020), algorithmic differentiation (Hieronymus et al., 2022), sensitivity studies (Saltelli, 2004; Montgomery, 2017) (for examples see Lohmann and Diehl (2006), Lohmann and Hoose (2009), Lohmann and Ferrachat (2010), Dedekind et al. (2021), and Ickes et al. (2022)). The following chapters in this work may serve as a case in point.

- **Generative entrenchment or path dependency** (Wimsatt, 2007; Lenhard and Winsberg, 2010; Winsberg, 2012; Babel, 2019) conceptualizes the fact that in the development of such a large model, presently available choices are restricted by past choices. The more complex the model, the more choices have gone into it, and the more restricted or time consuming are future implementations. This problem is exemplified by the development of a CCN climatology in Chp. 4. The quantities that need to be prescribed in a climatology are at least partially determined by the quantitites that the activation scheme needs as input (see Fig. 4.2).

- **Availability bias** may exaggerate the importance of processes that are represented (Guthke, 2017; Mülmenstädt and Feingold, 2018; Bender, 2020). While this phenomenon holds true for simple models as well, the complex models' increased authority may give a false sense of certainty, exacerbating the bias' effect.

- **Radically distributed epistemic agency** (Winsberg et al., 2014) means that no actor has ever been in a position to know about all methodological choices that went into the construction of a GCM and thus that no one is responsible for their results.

- **Distributed or sparse documentation** accentuates poor understanding and prompts mistakes (Menard et al., 2021).

- More detailed GCMs swamp scientists with more **output data**: "the more complex the model, the messier the garbage" (Heymann and Dahan Dalmedico, 2019, Frances Bretherton (quoted in Fisher (1988))).

- At the same time, climate models are relatively **easy to use**. The flow allows the modeler to set up a simulation easily, without understanding or even knowing what other programmers may have implemented, meant, switched on or adjusted (Lahsen, 2005; Dalmedico, 2007; Sundberg, 2009; Winsberg et al., 2014; Melsen, 2022).

Parker (2003) has put it pointedly: "determining why things happen as they do in complex model simulations is often very nearly as difficult as figuring out why things happen as they do in the real atmosphere". Thus, missing understanding of GCMs risks limiting their overall usefulness (Shackley et al., 1998).

Simplifications

> *Science may be described as the art of systematic oversimplification: the art of discerning what we may with advantage omit*
>
> — Shackley et al. (1998), citing Popper (1982) and Tennekes (1992)

While complexity has a firm stand in science, so does simplification. Models in particular "are useful precisely because they simplify the otherwise baffling complexity of the phenomena modeled" (Lahsen (2005), referring to Norton and Supper (2001)). Next to model expansion, radical pragmatism and drastic simplifications or approximations are also codes of climate modeling (Heymann, 2020). Thus modeling is always a question of where to draw the line for details[28].

The position of the line of course depends on the model's purpose, which may relax the constraint of realism (Rödder et al., 2020; Puy et al., 2022). In this work, we aim to reduce complexity that is underdetermined. We aim for model variants that are empirically equivalent in our purpose of modeling clouds in the climate system, yet simpler (Oreskes et al., 1994). Simplifications that remove unconstrained detail cater to all visions, as they enhance understanding and interpretability, leave results intact (while possibly allowing for time savings) and point out where representations are unconstrained. I attempt these simplifications in three parts (see Fig. 1.1). For the cloud microphysics scheme, I follow a bottom-up approach for process simplifications. Chapter 2 introduces a method to identify potential for simplifications in the cloud microphysics scheme of ECHAM-HAM. This method is then employed to two cloud microphysics schemes in Chapter 3. Indeed processes that the model is insensitive to are identified, and accordingly simplifications for these processes are suggested. For the aerosol module HAM, I attempt a top-down approach, testing radical simplifications of the whole module. In Chapter 4, the representation of aerosols entering the cloud microphysics scheme as CCN or INPs is simplified. The approach replaces the whole aerosol module HAM with climatologies for aerosol concentrations. Lastly, Chapter 5 discusses the results and common conclusions.

[28] As Gleick (1998) states: "The choice is always the same. You can make your model more complex and more faithful to reality, or you can make it simpler and easier to handle. Only the most naive scientist believes that the perfect model is the one that perfectly represents reality. Such a model would have the same drawbacks as a map as large and detailed as the city it represents. [...] Were such a map possible, its specificity would defeat its purpose: to generalize and abstract. [...] Whatever their purpose, maps and models must simplify as much as they mimic the world."

2

Assessing the potential for simplification in global climate model cloud microphysics

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Abstract Cloud properties and their evolution influence Earth's radiative balance. The cloud microphysical (CMP) processes that shape these properties are therefore important to represent in global climate models. Historically, parameterizations in these models have grown more detailed and complex. However, a simpler formulation of CMP processes may leave the model results mostly unchanged while enabling an easier interpretation of model results and helping to increase process understanding. This study employs sensitivity analysis of an emulated perturbed parameter ensemble of the global aerosol–climate model ECHAM-HAM to illuminate the impact of selected CMP cloud ice processes on model output. The response to the perturbation of a process serves as a proxy for the effect of a simplification. Autoconversion of ice crystals is found to be the dominant CMP process in influencing key variables such as the ice water path and cloud radiative effects, while riming of cloud droplets on snow has the most influence on the liquid phase. Accretion of ice and snow and self-collection of ice crystals have a negligible influence on model output and are therefore identified as suitable candidates for future simplifications. In turn, the dominating role of autoconversion suggests that this process has the greatest need

to be represented correctly. A seasonal and spatially resolved analysis employing a spherical harmonics expansion of the data corroborates the results. This study introduces a new application for the combination of statistical emulation and sensitivity analysis to evaluate the sensitivity of a complex numerical model to a specific parameterized process. It paves the way for simplifications of CMP processes leading to more interpretable climate model results.

2.1 Introduction

Aerosols and cloud microphysics (CMPs) control cloud properties and thereby exert a large influence on Earth's climate. For example, the cloud water and ice contents determine the cloud albedo and lifetime, and they also control precipitation formation (Mülmenstädt et al., 2015). In a changing climate, the correct representation of clouds is especially important to estimate Earth's radiation budget (Sun and Shine, 1995; Tan et al., 2016; Matus and L'Ecuyer, 2017; Lohmann and Neubauer, 2018). However, clouds and cloud feedbacks are a major source of uncertainty for projections of climate sensitivity in global climate models (Cess et al., 1990; Soden and Held, 2006; Williams and Tselioudis, 2007; Boucher et al., 2013).

Since cloud microphysical processes such as the riming of cloud droplets on snowflakes occur on scales much smaller than the resolution of global climate models (GCMs), they are parameterized; i.e., only their macroscopic effects at the scale of the model grid are described. Responding to the challenge of incorporating these processes in climate models, the community has added more and more processes into GCMs (Knutti and Sedláček, 2013) with increasing detail in their representation (e.g., Archer-Nicholls et al. (2021) and Morrison et al. (2020)). As Fisher and Koven (2020) argue for a similar situation in land surface modeling, this may be due on the one hand to scientists' tendency to focus on their own area of expertise. On the other hand, it also reflects the fact that the Earth system is indeed complex and that many processes may matter. However, it is doubtful whether more detail will help us to reduce uncertainty (Knutti and Sedláček, 2013; Carslaw et al., 2018). More complexity also has its downsides: more parameterized processes lead to more parametric uncertainty, which in turn scientists investigate and try to reduce with large scientific effort (e.g., Rougier et al. (2009), Lee et al. (2011), Yan et al. (2015), Williamson et al. (2015), and Dagon et al. (2020)). In fact, Reddington et al. (2017) argue that "aerosol–climate models are close to becoming an overdetermined system with many interacting sources of uncertainty but a limited range of observations to constrain them", referring to the complexity in the representation of aerosols and their interaction with clouds. This is related to equifinality, meaning that model versions from different regions of the input parameter space may lead to the same results that compare well with observations. These models may simulate a range of aerosol forcings (Lee et al., 2016), which is not possible to constrain with current observations. Morrison et al. (2020) diagnose the same problem for CMP schemes, whose complexity they say is "'running ahead' of current cloud physics knowledge and the ability to constrain schemes observationally". Climate models have become so complex that they are impossible to comprehend by any one scientist (Fisher and Koven, 2020). More detail means more heterogeneity between climate models, which increases the difficulty of a meaningful comparison of their projections (Fisher and Koven, 2020). But also within a given model, the attention and detail given to some cloud microphysical processes come at the expense of other less accessible processes. This brings the danger of overinterpreting those processes that are represented in detail while neglecting the impacts of poorly represented ones (Mülmenstädt and Feingold, 2018). Finally, the detail of the aerosol and cloud microphysics increases computational demand and thereby costs (though anticipating the results of Sec. 2.3.6, the four CMP processes investigated in this study require negligible computing time). It can thereby inhibit other advancements such as the move towards high-resolution simulations (which may themselves also require adaptations of the CMP schemes) or larger ensembles.

In contrast, simple models are easier to interpret and derive understanding from, as long as they represent processes correctly (Koren and Feingold, 2011; Mülmenstädt and Feingold, 2018). Also, assumptions and their consequences are more traceable in simpler or more system-oriented models (Mülmenstädt and Feingold, 2018). For example, conceptual cloud models have been used to investigate the impact of the choice of precipitation particle attributes on the cloud structure and evolution (Wacker, 1995) or to confirm microphysics findings qualitatively (Wood et al., 2009). Simplifications reduce computational demand, and simplified models yield themselves to other applications, e.g., the use in integrated assessment models (Ghan et al., 2013). At the same time, they may produce similarly good results as more complex models. For example, Ghan et al. (2012) developed a simple yet physical model for the aerosol indirect effect, whose estimates are comparable to those of complex global aerosol models. Similarly, Liu et al. (2012) compared two aerosol modules with seven and three lognormal modes and find that the simulated aerosol concentrations are remarkably similar.

The addition of detail and refinement of a model description is a natural response to the challenge of capturing something as complex as the climate system in a computer model. This is legitimate and beneficial. For example, it may lead to a physically more correct representation and reduce the number of tuning parameters (e.g., Storelvmo et al. (2008)). And for some applications modelers may need as much detail as possible in one specific module. Hence, scientists tend to call for more detail in process representations (e.g., Gettelman et al. (2013), for warm-rain microphysics; Sotiropoulou et al. (2021), for secondary ice production by break-up from collisions between ice crystals) instead of less. This may in part be because humans are biased towards searching for additive pathways as problem solutions while overlooking subtractive transformations (Adams, 2021). However, due to the reasons mentioned above, a simplified model equifinal to a more complex model may be more useful for gaining understanding of climate models (equifinal meaning that the two model versions lead to similar results). One can therefore question the need for an ever increasing amount of detail, especially in the face of overdetermination (Reddington et al., 2017). In this paper, we propose a new methodology to assess where process parameterizations can be stripped of detail to aid the development of a simplified model as well as to increase understanding of the model.

The role of CMPs within GCMs has been investigated previously: the influence of CMPs has been shown to dominate over that of aerosol schemes in affecting clouds and precipitation in the Weather Research and Forecasting model (White et al., 2017), as well as to dampen the influence of aerosol microphysics on cloud condensation nuclei and ice-nucleating particles in a regional model (Glassmeier et al., 2017). For the HadGEM-UKCA global aerosol–climate model, Regayre et al.

(2018) have shown that both aerosol and physical atmosphere parameters contribute to uncertainty in aerosol effective radiative forcing. Diving into the importance of single processes for the overall CMPs, Bacer et al. (2021) extracted process rates from the chemistry–climate model EMAC, which is based on the same CMPs as this study's ECHAM-HAM. They found that ice crystal sources in large-scale clouds are controlled by freezing and detrainment from convective clouds, while sinks are dominated by autoconversion and accretion. This approach is somewhat similar to a pathway analysis (e.g., Schutgens and Stier (2014) and Dietlicher et al. (2019)) in that it deepens understanding of immediate effects but is not able to relate the effect of a process on variables further down the process chain.

A promising method for investigating the effect of model input on output is the use of perturbed parameter ensembles (PPEs) (Murphy et al., 2004; Collins et al., 2011). In a PPE multiple input parameters are perturbed at the same time. In this way, PPEs expand upon sensitivity studies that vary one parameter (e.g., Lohmann and Ferrachat (2010) and He and Posselt (2015)) or multiple parameters at a time (e.g., Ghan et al. (2013)), allowing the investigation of the interaction effects of perturbations within the whole possible parameter space. For example, Sengupta et al. (2021) used a PPE to determine the impact of parameters related to secondary aerosol formation on organic aerosol in a global aerosol microphysics model. In a next step, parameter ranges can be constrained when comparing the PPE to observations (Posselt, 2016; van Lier-Walqui et al., 2014; van Lier-Walqui et al., 2019, note that these studies all used synthetic observations as constraints). Morales et al. (2021) built a PPE of CMP process parameters and environmental conditions, generated using a Markov chain Monte Carlo algorithm, in idealized simulations to then constrain the parameters with synthetic observations.

Another benefit is that a PPE does not require any additional changes to model code, in contrast to a pathway analysis that requires additional diagnostics and tracers. The downside is that PPEs require many simulations to sample the whole parameter space, which is prohibitive given the cost of global climate model simulations. A remedy is the combination of a PPE with a surrogate model such as an emulator. The emulator is first fitted to the PPE model output and then sampled instead of the GCM, which is expensive to run. This technique has been used, for example, to study the effect of model parameters such as the entrainment rate coefficient on climate sensitivity in a GCM (Rougier et al., 2009) or how model parameters affect forecast model drift (Mulholland et al., 2017).

Global sensitivity analysis is a method to quantify the effect of inputs on model output more formally. It allows us to divide the total variation in output into the direct contributions from variations in independent inputs as well as from their interactions. For example, Tan and Storelvmo (2016) used variance-based sensitivity analysis on a generalized model of their PPE to determine that the Wegener–Bergeron–Findeisen timescale is the most influential parameter in determining the cloud-phase partitioning in mixed-phase clouds. Bernus et al. (2021) have employed sensitivity analysis of their PPE directly to improve the understanding of their lake model prior to its implementation into a climate model.

When dealing with large models that are expensive to run, a surrogate model that is cheap to run allows for a tight sampling of the whole parameter space which permits for sensitivity analysis on the resulting surface. As such, the combination of a PPE with a surrogate model upon which sensitivity analysis is performed has found wide use in cloud simulation studies (Wellmann et al., 2018; Glassmeier et al., 2019; Wellmann et al., 2020; Hawker et al., 2021a). For example, Lee et al. (2011) emulated a global aerosol model and found that the cloud condensation nuclei concentration in polluted environments is dominated by sulfur emissions but that in remote regions interactions between different parameters are substantial. In particular, a range of recent studies has employed the methodology to investigate how uncertainty in input parameters (which are often not well constrained within parameterizations) translates to an uncertainty of climate model output: quantifying the effect of aerosol parameters on cloud properties or radiative forcing (Lee et al., 2011; Lee et al., 2012; Carslaw et al., 2013; Lee et al., 2013; Regayre et al., 2014; Johnson et al., 2015; Regayre et al., 2015; Yan et al., 2015; Regayre et al., 2018), but also in various other areas of environmental modeling (e.g. a land model in Dagon et al. (2020)). In a further step, the effect of an observational constraint on the model output can be investigated with the emulator as a surrogate model (Tett et al., 2013; Williamson et al., 2013; Lee et al., 2016; McNeall et al., 2016; Johnson et al., 2018), yielding important conclusions about which observations are needed to constrain climate models and on which parameters we need to focus research efforts. The approach also lends itself to an investigation of tuning parameters since these also form a parameter space that needs to be explored and constrained (Williamson et al., 2015; Hourdin et al., 2020; Couvreux et al., 2021).

Here we propose a new application of the combined PPE and sensitivity analysis approach to learn about the needed accuracy in process parameterizations within GCMs. Instead of varying parameters within parameterizations, we perturb the processes themselves as a whole. By perturbing we mean that we vary the effectiveness of a given process, going from using 50 % to 200 % of a process's effect in the model. For example, if a process affects the ice crystal number concentration, the change induced on it is multiplied by a perturbation factor between 0.5 and 2 in each time step. This means that in the extreme cases it would produce half or twice the effect on the ice crystal number concentration that it has in the default model (see Sec. 2.2.2 for further detail). From the resulting response surface we infer the sensitivity of model output to the CMP processes. The thus generated understanding points to processes whose representation needs to be accurate since they have a large influence and suggests simplifying those processes that have little influence on model output. Accepting the notion of equifinality, we aim to identify the parts of our current model that do not contribute to variation in output. Thus, we develop a "global sensitivity analysis that can weed out unimportant parameters" as called for by Qian et al. (2016).

To avoid misunderstanding: we are using a surrogate model to learn about sensitivities within the ECHAM-HAM GCM. We are not aiming to replace CMP parameterizations with machine learned substitutes (as e.g., Seifert and Rasp (2020)) or substitute model components (e.g., Beusch et al. (2020)) because interpretable, physics-based models should be preferred (Rudin, 2019). Instead, in line with Couvreux et al. (2021) we are using emulation and sensitivity analysis as a tool to generate understanding that allows us to build a more interpretable model version in a second step. Please note that the potential for simplification is evaluated in the current climate. Thus, any derived simplifications would need to be evaluated against a reference model for their suitability in a changed climate state prior to employing it in, e.g., climate change projections.

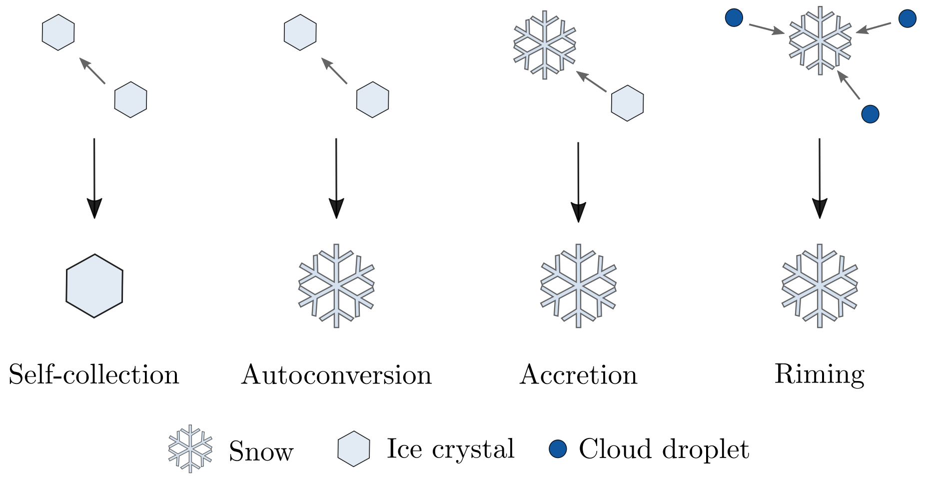

Figure 2.1: The four cloud microphysical processes investigated in this study, depicted as they are represented in ECHAM-HAM.

In Sec. 2.2 the CMP processes that we investigate, their treatment in the ECHAM-HAM GCM, the generation of the PPE and emulator, and the sensitivity analysis are described. In Sec. 2.3 the results from a "one-at-a-time" sensitivity study that explores the axes of the parameter space (Sec. 2.3.1), the emulated PPE (Sec. 2.3.2), and the sensitivity study on the fully sampled parameter space (Sec. 2.3.3) including a scale dependency (Sec. 2.3.4) and seasonal analysis (Sec. 2.3.5) are presented and discussed. Conclusions and an outlook are given in Sec. 2.4.

2.2 Methods

2.2.1 Cloud Microphysics in ECHAM-HAM

This study employs the global aerosol–climate model ECHAM6.3-HAM2.3 (Tegen et al., 2019; Neubauer et al., 2019), with a T63 horizontal spectral resolution and 47 vertical levels. The cloud microphysics consist of a two-moment prognostic scheme for ice crystals and cloud droplets, with additional one-moment prognostic representation of snow and rain (Lohmann and Roeckner, 1996; Lohmann et al., 1999; Lohmann, 2002; Lohmann et al., 2007; Lohmann and Hoose, 2009; Lohmann and Neubauer, 2018). The stratiform cirrus scheme includes homogeneous nucleation of supercooled liquid droplets (Kärcher and Lohmann, 2002b; Kärcher and Lohmann, 2002a; Lohmann, 2003). The stratiform liquid cloud scheme encompasses condensation, aerosol activation, autoconversion of cloud droplets to rain, accretion of cloud droplets by rain, evaporation of cloud and rainwater, and wet scavenging of aerosol particles (for further details and references see Neubauer et al. (2019)). In stratiform mixed-phase clouds, various CMP processes are included: heterogeneous nucleation via immersion and contact freezing, depositional growth of cloud ice, growth of ice crystals at the expense of cloud droplets via the Wegener–Bergeron–Findeisen process (Wegener, 1911; Bergeron, 1935; Findeisen, 1938), and sublimation and melting of ice crystals and snow below clouds. In this study, we are investigating the effect of four different CMP processes involving the ice phase (see Fig. 2.1). **Self-collection** of ice is the process of ice crystals sticking together to form a single ice crystal. **Autoconversion** also has two ice crystals sticking together, albeit forming a snowflake.

In **accretion**, a snowflake collects an ice crystal, resulting in a larger snowflake. The fourth process is the only one involving the liquid phase: cloud droplets are **riming** on a snowflake, again enhancing its size. The implementation of these processes in terms of changes to the ice crystal and cloud droplet mass is detailed in Lohmann and Roeckner (1996), while the implementation of changes to the ice crystal and cloud droplet number concentration is simply in proportion to the mass changes (except for where the mass concentration is unaffected; Lohmann et al. (1999) and Lohmann (2002)). The distinction between accretion and autoconversion is necessary due to the separation between ice crystals and snowflakes in their representation as categories of ice in the model. Snowflakes precipitate, while ice crystals are smaller and sediment but do not survive outside clouds. The four processes were chosen for their comparability, as they all represent particle interactions, to represent a range of assumed impacts, as well as for their implementation, which is clearly distinguishable in the code and allowed for easy implementation of the perturbations (see Sec. 2.2.2). In this study, we do not include any ice multiplication processes. Convective clouds are treated separately from stratiform clouds, except for the interaction through detrained condensate from convective clouds, which is added to stratiform clouds if they exist at the respective model level.

Apart from the perturbations described in the next section, substantial changes that were applied with respect to the published model version ECHAM6.3-HAM2.3 (Neubauer et al., 2019) are the following.

- Detrained condensate from the convective cloud scheme produced an unrealistically large amount of ice crystals at mixed-phase temperatures, which were then removed with a correction term. The detrained cloud particles are now assumed to be all liquid at mixed-phase temperatures ($0\,°\mathrm{C} < T < -35\,°\mathrm{C}$; Dietlicher et al. (2019) and Muench and Lohmann (2020)).

- In line with Muench and Lohmann (2020, Sec. 3.3.1.2), we now include the immediate, updraft-dependent self-collection of detrained ice crystals.

- Previously, a fixed minimal cloud droplet number concentration (CDNC) was applied, which led to unrealistically high CDNCs in high-latitude and/or high-altitude clouds with low liquid water content (LWC) and hence small droplets. We replace this with a dynamically calculated minimal CDNC, which is calculated from the in-cloud water content and a set maximum volumetric cloud droplet radius (set at 15 µm in the simulations conducted for this study). The resulting minimum CDNC needs to lie between $10 \times 10^6\,\mathrm{m}^{-3}$ and $4 \times 10^7\,\mathrm{m}^{-3}$. Admittedly, we are replacing the tuning parameter of fixed minimum CDNC with one for a maximum cloud droplet radius. The latter is preferred as it is more physical.

- The model version of Neubauer et al. (2019) contains a mistake in the calculation of the hygroscopicity parameter in the aerosol activation parameterization, leading to an underestimation of the individual aerosol-mode solubility. The calculation was updated in Friebel et al. (2019) and subsequently used in Lohmann et al. (2020); this correction is also applied here.

- In part motivated by the large correction terms highlighted in the process rate study of Bacer et al. (2021) we reduce these if they are unnecessary and/or unphysical. For example, conditions of maximum ice crystal number concentration (ICNC) were enforced after a few CMP processes took place in Bacer et al. (2021). We could reduce the value of that correction term by applying it after each relevant process. Most importantly, the diagnosis of multiple correction terms acting on the same variable led to an artificial increase in corrections. For example, correction terms would enhance ICNC concentrations at model points that later were identified to be outside a cloud (due to the way the code is structured, the diagnosis of cloud cover happens after, e.g., activation/nucleation takes place). In turn, ICNCs outside a cloud were then corrected to be zero, so an unnecessary correction was in fact counted twice. We reduce this artifact by correcting the correction terms themselves. Staying with the example above, the first correction term is now itself set to zero outside a cloud.

- The sublimation of sedimenting ice crystals appears to be too weak in ECHAM-HAM. This became apparent as in-cloud ICNCs were increasing through sedimentation from above, which indicates that sublimation of ice crystals falling into the cloud-free part of a grid box is too weak. While the underlying problem of a weak sublimation needs to be addressed with future efforts, we introduced a correction of the sedimentation routine: the gain of ice crystal concentrations in the level k into which the ice crystals sediment, $\Delta\mathrm{ICNC}_{\mathrm{sed},k}$, is restricted to the loss of in-cloud ice crystal number concentration in the lowest model level above level k that lost ice crystals by sedimentation. Also, in-cloud ICNC and the snow formation rate are now set to 0 outside clouds inside the ice crystal sedimentation routine wherein they were previously set to the grid-mean values. This contains the implicit assumption that ice crystals do not survive sedimentation outside a cloud in ECHAM-HAM.

With the described changes, the model requires retuning. The tuning procedure follows the one described in Neubauer et al. (2019), with the final tuning parameters given in Table A.1 in Appendix A.1. Model simulations were conducted with the same tuning for all simulations.

2.2.2 Perturbations as a proxy for complexity

In order to see the effect of whole processes on model output, we can turn processes off in sensitivity studies. In the present study, we achieve this by setting the change that the process induces on prognostic variables to zero. For example, at every model time step t autoconversion impacts the ICNC:

$$\mathrm{ICNC}_{t+1} = \mathrm{ICNC}_t + \Delta\mathrm{ICNC}_{\mathrm{autc}}. \tag{2.1}$$

We can turn off the effect of autoconversion by multiplying $\Delta\mathrm{ICNC}_{\mathrm{autc}}$, the change in ICNC due to autoconversion in one time step, by zero when it is added to the affected variables.

More generally, instead of setting the changes induced by a process to zero, we can perturb the process using a newly defined parameter η.

$$\mathrm{ICNC}_{t+1} = \mathrm{ICNC}_t + \eta_{\mathrm{autc}} \cdot \Delta\mathrm{ICNC}_{\mathrm{autc}} \tag{2.2}$$

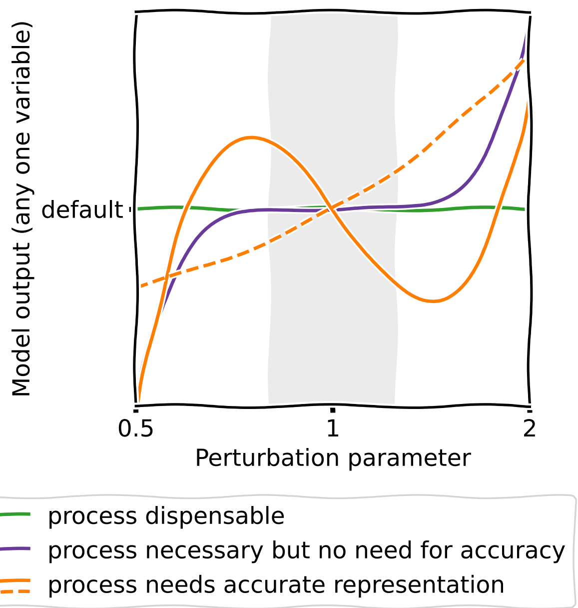

Figure 2.2: Sketch of the envisioned interpretation. The shading indicates the area that is of most interest to judge the effect of process simplifications on the model output. If the slope in this area is small, this suggests that the process can be simplified (green and purple lines). A large slope indicates that the process needs to be represented accurately (orange lines). If no perturbations of the process in the 0.5 to 2 perturbation parameter range and the suppression of the process (perturbation parameter of 0, not shown) have a significant influence on the model output, the process may be removed entirely (green line).

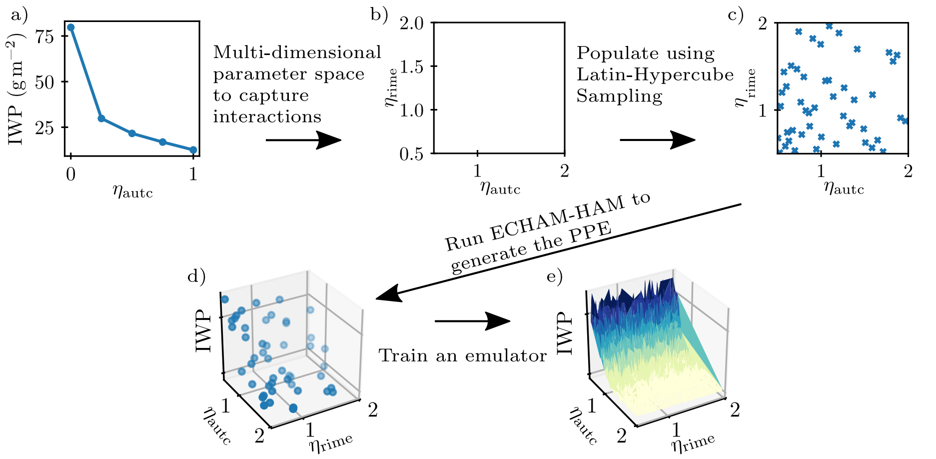

Figure 2.3: Sketch of the employed methodology: we move from **(a)** one-dimensional sensitivity studies wherein one process is perturbed by varying the parameter η (Sec. 2.3.1) to **(b)** a multidimensional parameter space. **(c)** The input parameter space is filled with Latin hypercube sampling and supplied as input to ECHAM-HAM. The simulations form the perturbed parameter ensemble (PPE). The **(d)** PPE output is **(e)** fitted using a Gaussian process emulator for each variable of interest to generate a smooth response surface, upon which sensitivity analysis can be applied. Note that this is an illustrative sketch of the method for a PPE with two input dimensions, whereas our PPE has four dimensions, and that the data used to generate it are only illustrative as well. The shading in **(d)** illustrates depth only.

This perturbation of whole processes was introduced by van Lier-Walqui et al. (2014) to estimate the uncertainty including errors in the physical assumptions of process formulations. In our case, the parameters aid understanding the sensitivity of the model to each process: from the response of model output to variations in η_i, we can extract information on how accurately a process i needs to be represented in the model (see Fig. 2.2 for a visualization). For example, if the model output variable (e.g., ice water path, IWP) as a function of η_i has a slope close to zero at $\eta_i = 1$ (green and purple line in Fig. 2.2), this suggests that the process i needs to be represented only approximately and that some detail could probably be removed from its parameterization without much of an effect on the model performance. Note that the perturbations are constant in space and time for each PPE member, serving as a proxy for understanding the effect of possible simplifications, which would likely be variable in time and space. In this study, four cloud microphysical processes, namely self-collection, autoconversion, accretion, and riming (see Fig. 2.1), are perturbed, i.e., $i \in [1, 4]$. Combining perturbations of multiple processes allows us to study and take into account possible interaction effects, such as the compensation by one process which is perturbed by another one.

2.2.3 Generating and emulating the perturbed parameter ensemble (PPE)

In a first scoping study, we perturb each process one by one by multiplying its effect with $0 < \eta_i < 1$. Multiplicative perturbations between zero and 1 correspond to a reduction in the effectiveness of the process. However, to take into account interactions, all η_i values need to be varied at the same time, thereby creating a multidimensional input parameter space in a second step. In addition, the range of η_i is expanded to values up to $\eta_i = 2$ to imitate an overestimation of a given process due to an inaccurate description. As we are most interested in the space around $\eta_i = 1$, and to sample the over- and underestimation equally, we vary η_i from 0.5 to 2 in the multidimensional input parameter space. If the process uncertainty were known, it would influence the extent of the perturbation range, which could be different for each process. The perturbations and the procedure described in the following are visualized in Fig. 2.3. To probe the multidimensional input parameter space effectively, the sets of input parameter combinations (η_1, η_2, η_3, η_4) to be simulated with the model were generated with Latin hypercube sampling (LHS, using the Python library PyDOE, tisimst (2021)), which maximizes the spacing between inputs and provides good coverage of the parameter space, even when only a few input parameters are important (Morris and Mitchell, 1995). The LHS was applied to the logarithmically scaled input range to account for the multiplicative behavior of the η_i. Each of the LHS-generated input combinations was then used as input for a 1-year ECHAM-HAM model simulation, creating a perturbed parameter ensemble (PPE) with 48 members. This is in line with the suggestion of Loeppky et al. (2009) to use 10 times as many training runs as the number of input parameters for such a computer experiment. To estimate the interannual variability, the control simulation with all processes at full effectiveness ($\eta_i = 1 \forall i$) spanned 10 years. This estimate is used to judge whether perturbations observed in the PPE are significantly larger than the interannual variability and therefore contain a signal that originates from the perturbation in η_i. As the interannual variability exhibited no strong variations throughout the probed phase space in the one-at-a-time sensitivity studies, the 1-year simulations for the PPE members in combination with the control simulation estimate of the variability were deemed sufficient for the analysis. All the simulations were performed with climatological sea surface temperatures and sea ice extents, as well as aerosol emissions representative for the year 2003. These simulations were not nudged to meteorological data but ran freely so that the full effect of perturbing the processes could be observed. Each simulation included 3 months of spin-up that was not included in the analysis.

Using the PPE output as input for the creation of a surrogate model, we can construct a smooth response surface over the whole parameter space (see Fig. 2.3e). As a surrogate model, we choose a Gaussian process emulator (O'Hagan, 2006; Rasmussen and Williams, 2006), which has found wide use in atmospheric and climate science (Lee et al., 2011; Carslaw et al., 2013; Johnson et al., 2015). We prefer the Gaussian process emulator over, e.g., a neural network because of its demonstrated suitability and need for fewer input data (see Watson-Parris et al., 2021a, for a more in-depth discussion). Using a recent Python package for emulating Earth system models (Watson-Parris et al., 2021c; Watson-Parris et al., 2021a), the implementation is straightforward. From the PPE, we can construct a surrogate model for every output variable that we are interested in by training a separate emulator for each output variable (ice crystal and cloud droplet number concentration, ice and liquid water path, shortwave and longwave cloud radiative effect, cloud cover, surface precipitation, ice, liquid, and mixed-phase cloud cover). For the kernel (or covariance function, Watson-Parris et al., 2021a), an additive combination of the linear, polynomial, bias, and exponential kernels was used as this performed best in preliminary tests (not shown, Duvenaud (2014)). Other model specifics were

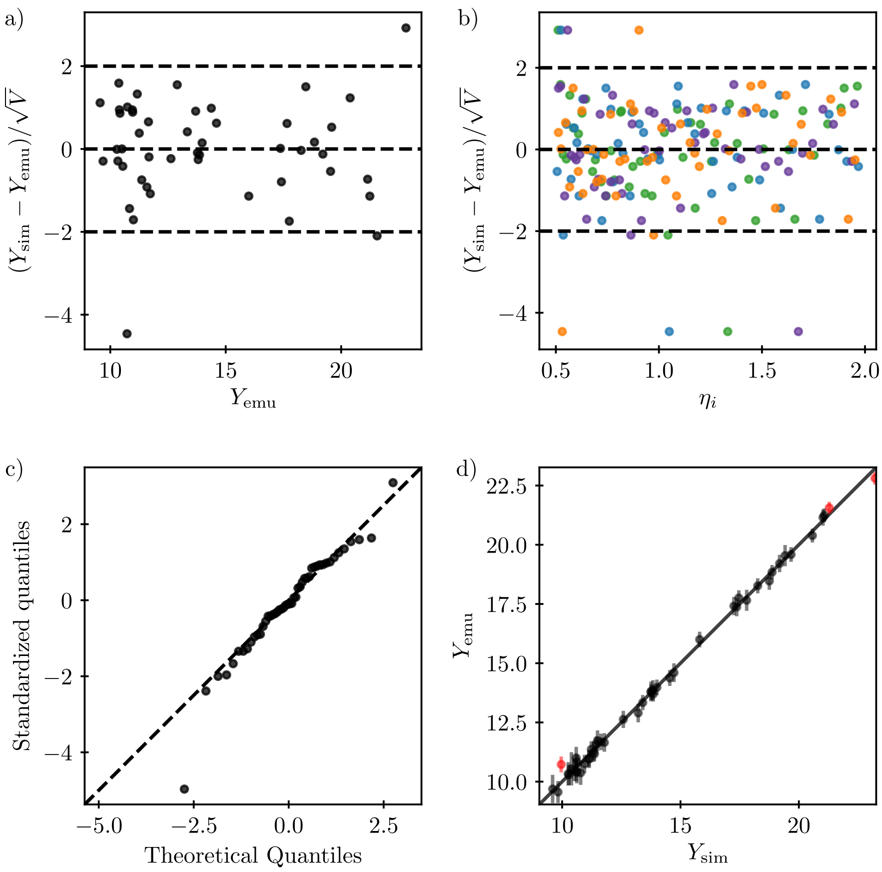

Figure 2.4: Leave-one-out validation of the emulator for global annual mean IWP. Each point corresponds to the training of the emulator on all points except one and then testing on exactly that point. Individual standardized errors are plotted against **(a)** emulator output and **(b)** input parameters (colors according to Fig. 2.5: autoconversion – blue, accretion – purple, riming – green, self-collection – orange). The dashed lines are drawn at an individual standardized error of zero and 2, which is the threshold discussed in Bastos and O'Hagan (2009). **(c)** QQ-plot of the individual standardized errors against a Student's t distribution. **(d)** Emulator against model output, with the error bars indicating the 95 % confidence interval on the emulator predictions. Predictions for which the model result lies outside that interval are marked red.

set as default in Watson-Parris et al. (2021c). As the emulation operates best on standardized data with zero mean and unity variance, the mean was removed from the input data, which was then scaled by dividing it by the standard deviation, prior to emulation. With the cheap surrogate model a variance-based sensitivity analysis (see Sec. 2.2.5) becomes feasible (Oakley and O'Hagan, 2004), picking 3000 samples from the emulator as input. This approach is similar to Johnson et al. (2015), except that they perturbed CMP parameters, while we vary the effectiveness of whole CMP processes. It allows us to identify the importance of the different η_i for the variables in question and thereby the processes which require a detailed representation.

2.2.4 Validation

To make sure that the chosen emulators are a fair representation of the model output, we validate them according to Bastos and O'Hagan (2009) except for using leave-one-out validation, as visualized in Fig. 2.4 for the IWP. In Fig. 2.4a and b, the individual standardized errors, $\frac{Y_{\mathrm{sim}}-Y_{\mathrm{emu}}}{\sqrt{V_{\mathrm{emu}}}}$ (with Y_{sim} and Y_{emu} as the output of the ECHAM-HAM simulations and the emulated output, respectively, and V_{emu} the emulator variance), are plotted against the emulated output and input parameters. We observe only a few errors larger than 2, which would signal a conflict.

We employ a QQ-plot to determine whether the normality assumption of a Gaussian process is met in the emulator (Bastos and O'Hagan, 2009). The plot compares the quantiles of the standardized errors against those of a Student's t distribution. Figure 2.4 c indicates that the normality assumption holds and that the predictive variability is well estimated by the emulator (Bastos and O'Hagan, 2009). In a direct comparison of emulated and simulated ECHAM-HAM model output (Fig. 2.4d), the points should lie close to the line of equality, with the 95 % confidence bounds on the emulator predictions crossing it. This should be the case for 95 % of the validation points. In our emulations, the number of points with confidence bounds that do not cross the line of equality is sometimes larger (up to 27 %), depending on the variable. We attribute this to the disruptive changes that the CMP process perturbations induce compared to, e.g., the aerosol and CMP parameter changes applied by Johnson et al. (2015) (which did not include ice crystal autoconversion and perturbed parameters only within uncertainty bounds instead of whole processes), as well as to the fact that the simulations were not nudged. The difficulty in emulating the response surface for some of the variables was also apparent in computational limitations: some of the leave-one-out validation emulations were not possible to compute because of numerical instabilities in the computations when constructing the emulator. As these were only a few cases (up to two for global means and four for seasonal means in 48 validation emulations), the validation for those variables as a whole is still deemed valid.

The good qualitative agreement with the line of equality and the lack of systematic errors are sufficient for a validation of the emulator, especially considering that we are not aiming for exact quantitative estimates as results of the presented analysis. Rather, we are looking for a conceptual understanding of the need for an accurate description of CMP processes, for which this emulator validation is sufficient.

For the variables which passed the leave-one-out validation, the final emulator used for the sensitivity analysis was trained on all PPE members (note that in a few cases only 47 PPE members were used due to numerical instabilities in the computations when constructing the emulator). Note that the setup of the emulator includes design choices such as the kernel combination to use. Therefore, the present emulator is only one of multiple possible emulators that could be used to represent the model data. However, as it is shown to validate well, other setups are expected to lead to the same conclusions as this one in the analysis.

2.2.5 Sensitivity analysis

In our framework, the question of how detailed the representation of a given process i needs to be translates to the question of how sensitive the model output is to a variation of the perturbation parameter η_i. For an answer, we employ variance-based sensitivity analysis, following Saltelli (2008a). In contrast to derivative-based local methods (Errico, 1997), global variance-based sensitivity analysis allows for an investigation of sensitivities within the whole input parameter space. Its main metrics are the first- and total-order sensitivity indices ($S_{1\mathrm{i}}$ and S_{Ti}, respectively). The first-order sensitivity index of η_i measures the contribution of variance in η_i to the variance in an output variable Y. It is constructed as

$$S_{1\mathrm{i}} = \frac{V_{\eta_i}\left(E_{\eta_{\sim i}}\left(Y|\eta_i\right)\right)}{V(Y)} \tag{2.3}$$

E is the average over Y with all η except η_i ($\eta_{\sim i}$) being allowed to vary while η_i is kept fixed at η_i^*. Then V_{η_i} is the variance over that average for varying η_i^*. $S_{1\mathrm{i}}$ is always between 0 and 1, and high values signal an important variable. For additive models all first-order terms add up to 1, i.e., $\sum_i S_{\eta_i} = 1$. In non-additive models (e.g., a climate model) interaction terms also have to be taken into account. However, in models with many input parameters the computation of all interaction sensitivities can be cumbersome. The total effect sensitivity index S_{Ti} offers a remedy in that it summarizes all direct and interactive effects a parameter's variance has on the total variance in output (Homma and Saltelli, 1996; Saltelli, 2008a). It is defined as

$$S_{\mathrm{Ti}} = \frac{V_{\eta_{\sim i}}\left(E_{\eta_i}\left(Y|\eta_{\sim i}\right)\right)}{V(Y)} \tag{2.4}$$

Here all but η_i ($\eta_{\sim i}$) are kept fixed at $\eta_{\sim i}^*$ and only η_i is allowed to vary for the average E_{η_i}. Then the variance of that average over varying $\eta_{\sim i}^*$ is computed and divided by the variance in output Y. Saltelli et al. (1999) argue that the first and total sensitivity index suffice for a meaningful global sensitivity analysis. To compute these indices via the Sobol method, we make use of the Python library SALib (Herman and Usher, 2017).

2.3 Results and discussion

2.3.1 One-at-a-time sensitivity studies

In a first scoping experiment, we perturbed each process separately, which one can imagine as tracing the edges of the cube shown in Fig. 2.3. The results are presented in Fig. 2.5. Of the four perturbed processes, turning off autoconversion has the largest effect on model output: the global annual mean ice water path (IWP) is more than doubled, and the increase in cloud cover and decrease in precipitation dwarf the changes induced by turning off the other three processes. In fact, the perturbations induced by perturbing accretion and self-collection are mostly insignificant compared to the interannual variability. As autoconversion is a removal process for ice crystals, it is reasonable that its suppression leads to an increase of ice in the atmosphere (note that the IWP in ECHAM-HAM only counts ice crystals and not snow). Similarly, riming is a removal process for liquid droplets, so the liquid water path (LWP) increases with its suppression. However, surprisingly the suppression of autoconversion induces a similarly large increase in LWP as that of riming, even though autoconversion includes no direct interaction with liquid droplets. The shape of the model response to the gradual perturbation of the processes holds additional information: while the generated model response is mostly gradual, for low η_{autc} the response is more abrupt. This behavior, which we call a threshold response, is most striking for the global annual mean LWP, for which the signal for $\eta_{\mathrm{autc}} \geq 0.25$ is not

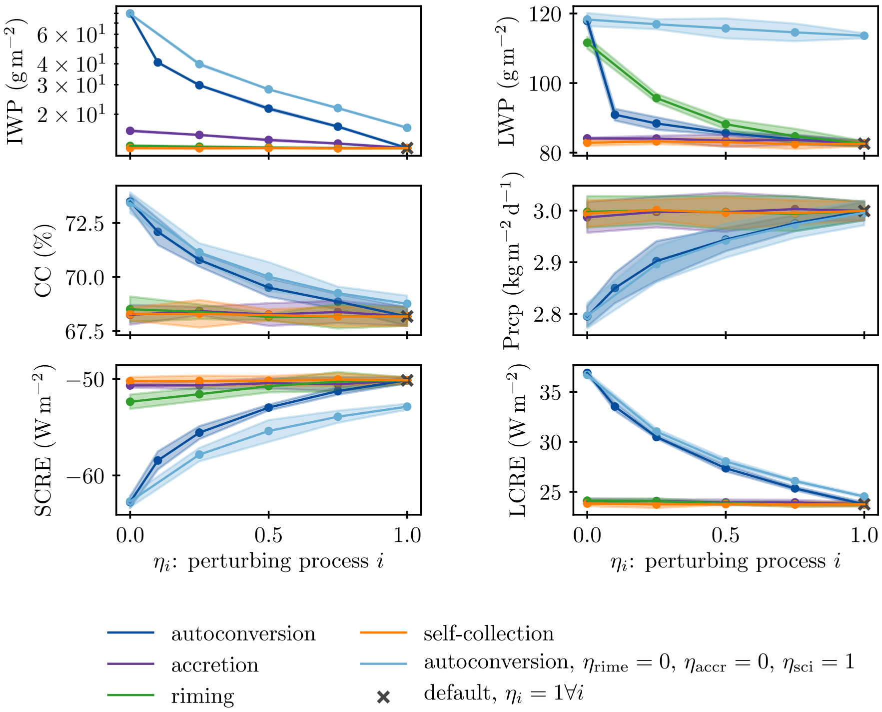

Figure 2.5: Model response to perturbations of four CMP processes: autoconversion, accretion, riming, and self-collection (as illustrated in Fig. 2.1) in terms of global annual mean IWP, liquid water path (LWP), cloud cover (CC), precipitation (Prcp), and short-wave and longwave cloud radiative effect (SCRE, LCRE). An additional experiment was conducted to highlight interactive effects between the perturbation of autoconversion and the suppression of riming and accretion (light blue). The points and line indicate the mean, and the shading indicates 2 times the standard deviation of annual mean values of a 5-year simulation. Classical sensitivity studies would only show $\eta_i = 0$ and $\eta_i = 1$. Note that we added an extra simulation at $\eta_{\text{autc}} = 0.1$ to better illustrate the threshold behavior discussed in the text and that for the IWP the shading is hidden behind the lines.

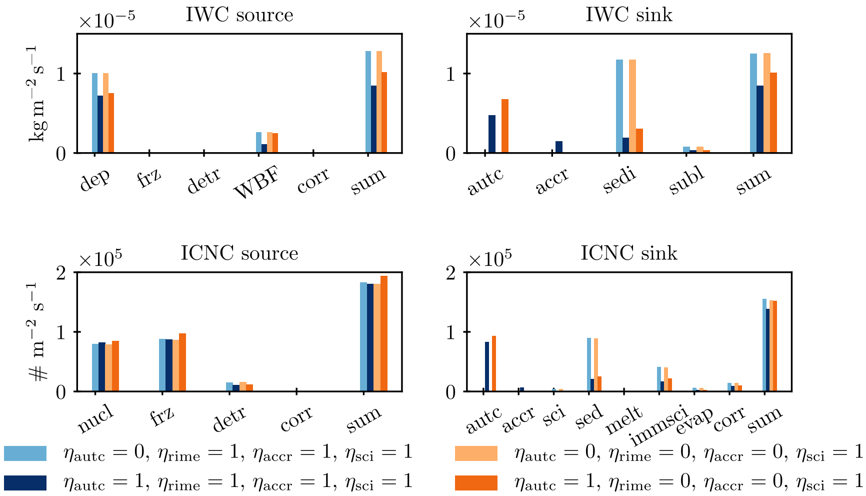

Figure 2.6: Global annual mean vertically integrated process rates for four experiments that illustrate the suppression of snow formation through turning off autoconversion (mean of a 5-year simulation). The rates are diagnosed similarly to Bacer et al. (2021), but correction terms were themselves subtracted from process rates where appropriate, i.e., where the correction belongs to the logical entity of the process rate (see Sec. 2.2.1). The process rates are deposition (dep), heterogeneous and homogeneous freezing (frz), detrainment (detr), deposition in the Wegener–Bergeron–Findeisen process (WBF), correction terms (corr), autoconversion (autc), accretion (accr), sedimentation (sedi), sublimation (subl), ice nucleation in the cirrus scheme (nucl), melting (melt), immediate self-collection of ice crystals when the ICNC is larger than a maximal threshold (immsci), and evaporation (evap).

significantly different to that of accretion and self-collection. When autoconversion is completely suppressed, the LWP increases dramatically and the signal becomes stronger than that for riming, which had increased consistently and gradually. This behavior can be explained by autoconversion acting as a catalytic process for accretion and riming, creating a threshold behavior when it is turned off. As can be seen from Fig. 2.1 it is the only process that generates snowflakes. Accretion and riming need the snowflakes to be able to act upon them. Therefore, when autoconversion is turned off, accretion and riming are consequently suppressed as well. In this way, the suppression of autoconversion can strongly influence even the liquid phase. The simulations in which we perturb autoconversion while having riming and accretion turned off confirm this hypothesis (light blue line in Fig. 2.5): throughout most of the phase space, turning off accretion and riming reinforces the signal from phasing out autoconversion. However, when autoconversion is turned off, turning off accretion or riming does not change the model output any further. That is because they are both suppressed when autoconversion is turned off and does not generate any snow for them to act upon.

Figure 2.6 further elucidates the reaction of the model to a suppression of autoconversion: the snow formation rate decreases dramatically, and with increased ice concentrations in the atmosphere, the other removal processes of sedimentation and melting subsequently increase. Again the suppression of riming and accretion only influences the model output when autoconversion is active. When autoconversion is turned off, accretion and riming have no influence.

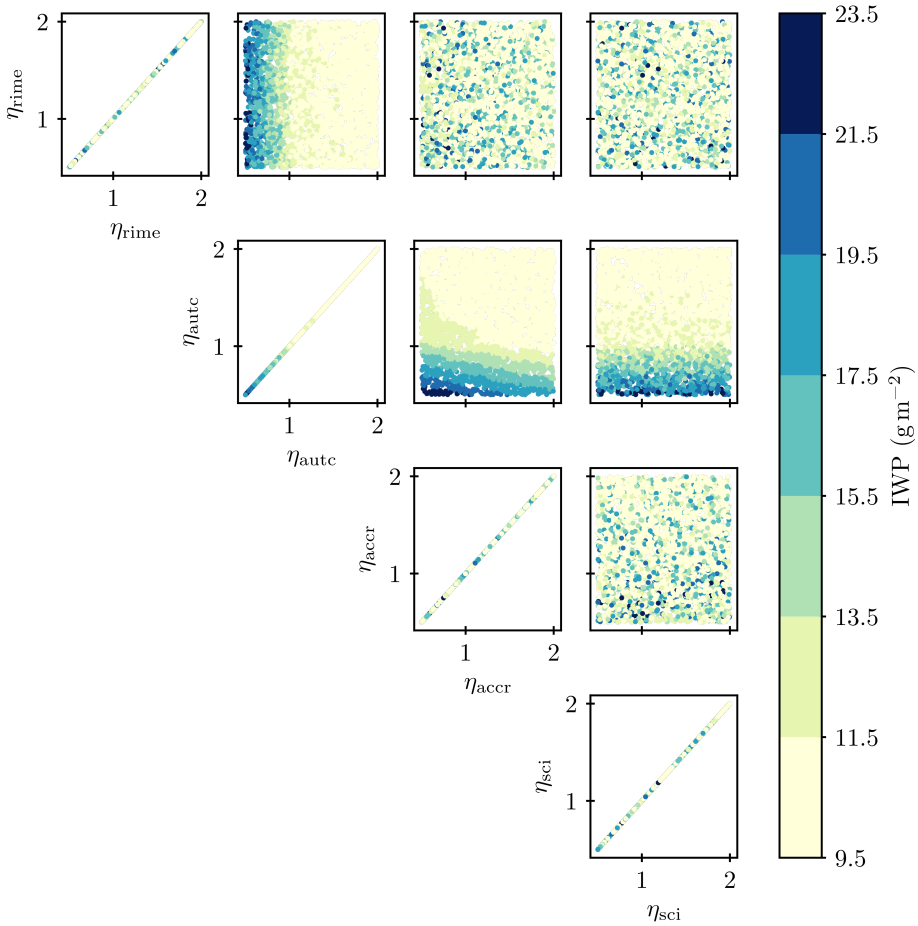

Figure 2.7: Two-dimensional projections of the IWP values sampled from the four-dimensional parameter space of the emulated PPE. Each perturbed process is a dimension, and the color bar denotes the global annual mean ice water path for each input parameter combination.

From this one-at-a-time example, one can already see the benefit of the perturbation approach: in classical sensitivity studies, wherein processes are only turned on and off, only the large signal induced by autoconversion would have been visible. However, here it was the peculiar shape of the model response to the whole perturbations that hinted at the threshold effect of autoconversion. The implications for possible simplifications are different: seeing only the large difference between a simulation with and without autoconversion, one would think that this is an immensely important process. Recognizing it as a threshold process and seeing the gradual response to small deviations from 1.0 in η_{autc} (similar to the purple curve in Fig. 2.2), it appears that there is potential for a less accurate description of autoconversion in the model. It has also become clear that interaction effects need to be taken into account as well to explain the model behavior. This is what the PPE expands upon in the next section.

2.3.2 PPE of global mean variables

Conducting a 1-year simulation with ECHAM-HAM for each of the 48 input parameter combinations generates the PPE which is then emulated (see Fig. 2.3). Figure 2.7 illustrates the resulting response surface with points sampled from that emulation of

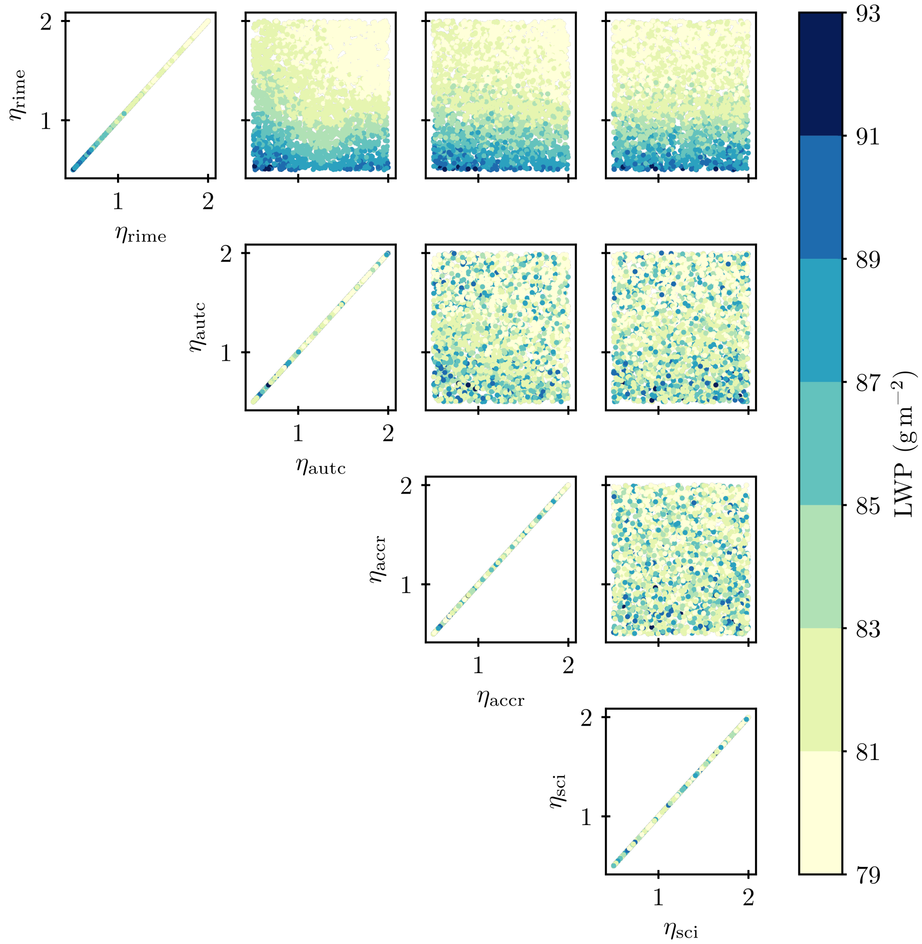

Figure 2.8: Same as Fig. 2.7 but for the global annual mean liquid water path. Results for additional variables are presented in Fig. A.1 in Appendix A.2.

the annual global mean IWP. To generate the multidimensional response surface 48 1-year simulations were needed compared to the 21 simulations that were needed to investigate the response along only a few of the parameter space edges in Sec. 2.3.1. This illustrates the value of the chosen approach: the emulated PPE provides more information while needing only roughly twice as many simulations. The surface shows an ordered ascent with decreasing η_{autc}, while the other dimensions exert no control over the value of the IWP. Only for accretion is a slight influence visible from the tilted contours in the phase space shared with autoconversion. Increased accretion depletes the IWP since it converts ice crystals to snowflakes. Figure 2.8 shows that the LWP is dominated by η_{rime}, with an additional influence of autoconversion. The LWP decreases with increasing η_{rime} and increasing η_{autc}. This is because riming depletes the atmosphere of cloud droplets and a decrease in autoconversion suppresses riming. The panels in Figs. 2.7 and 2.8 exhibiting no order in their parameter space distribution indicate that the processes in question exert no influence on the respective output variable. Similar to the LWP, the CDNC is dominated by riming, and for other cloud variables the dominant influence of autoconversion is confirmed as well (see Fig. A.1 in Appendix A.2).

The ranges in the global annual mean model variables that we observe are mostly larger than what Lohmann and Ferrachat (2010) find for varying uncertain tuning parameters, indicating that whole processes exhibit a larger influence on the model response than those single parameters. Only for LWP do Lohmann and Ferrachat (2010) find a larger range of about $50\,\mathrm{g\,m^{-2}}$ when they multiply the autoconversion rate with a factor between 1 and 10. As this warm-rain process is not included in the present analysis, it is reasonable that the observed variation for LWP is smaller.

2.3.3 Sensitivity analysis

A global variance-based sensitivity analysis allows us to quantify the qualitative sensitivities obtained from the graphical representations of the emulated surfaces in the previous section. The results for the first-order ($S_{1\mathrm{i}}$) and total effect (S_{T}) sensitivity indices are presented in Fig. 2.9. Indeed, the qualitative results are confirmed: the global annual mean LWP and CDNC are dominated by riming, while all other variables are dominated by autoconversion in both first-order and total effect.

The observed sensitivities are different from what Bacer et al. (2021) find in their investigation of EMAC ICNC process rates. They find that autoconversion contributes about twice as much as accretion to the ICNCs, while self-collection has a negligible role. In our analysis, the influence of autoconversion dwarfs that of accretion in terms of sensitivity indices as well as for the process rates (see Fig. 2.6). The sensitivity indices are not directly comparable to Bacer et al. (2021). However, for the default simulation the process rates are diagnosed as in Bacer et al. (2021) and thus comparable. We attribute the observed differences to the slightly different model version used in Bacer et al. (2021), which goes along with a different tuning.

The almost binary results for the sensitivity indices are surprising, as in other studies the sensitivity indices were more evenly distributed (Lee et al., 2011; Wellmann et al., 2018; Wellmann et al., 2020). However, these studies usually employed a wider suite of input parameters, whereas here only processes from the limited system of ice particle interactions are included. We expect that with additional cloud mi-

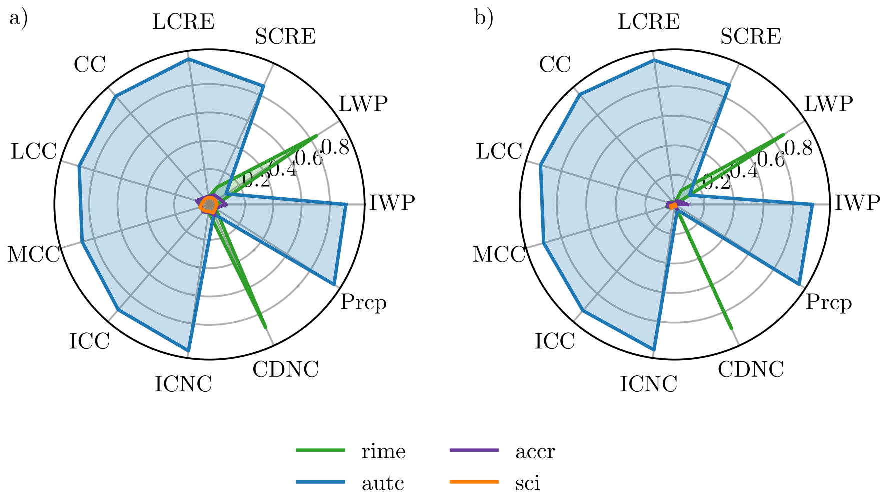

Figure 2.9: First-order **(a)** and total effect **(b)** sensitivity indices for the emulated response surface of global annual mean cloud cover (CC), liquid cloud cover (LCC, $T > 0\,°\mathrm{C}$), mixed-phase cloud cover (MCC, $0\,°\mathrm{C} < T < -35\,°\mathrm{C}$) ice cloud cover (ICC, $T < -35\,°\mathrm{C}$), longwave cloud radiative effect (LCRE), shortwave cloud radiative effect (SCRE), liquid water path (LWP), ice water path (IWP), and total precipitation. As described in Sec. 2.2.5, the indices are always between 0 and 1, and high values signal an important variable. Since the climate model is non-additive, the terms do not add up to 1 as interactions have to be taken into account.

crophysical processes included, the sensitivities would be more evenly distributed as well. The binary signal is due to the strong dominance of autoconversion throughout the parameter space and not due to the threshold behavior upon suppression of autoconversion as analyzed in Sec. 2.3.1. This was excluded from the sensitivity analysis as only the input parameter space with $\eta_{\mathrm{autc}} \geq 0.5$ was taken into consideration.

The dominance of autoconversion is hypothesized to originate from the nonlinearity in its parameterization. In contrast to the other processes, the conversion rate of autoconversion has a squared dependency on the cloud ice content (see Lohmann and Roeckner (1996)), increasing feedback effects between the two.

Additional reasons for the large role of autoconversion may lie in its role as a tuning parameter in ECHAM-HAM. For tuning, uncertain parameters of the model are used (Neubauer et al., 2019). Historically, the scaling factor for the stratiform snow formation rate by autoconversion, γ_{s}, has been used as it represents a counterpart to the scaling factor for the stratiform rain formation rate by autoconversion. To reach the tuning goals as detailed in Neubauer et al. (2019), it is brought to unrealistically high values (see Table A.1). This enhances the changes induced by perturbing autoconversion in this study using η_{autc}. Additionally, structural problems in the model may enhance the role of autoconversion artificially. For example, by accounting for heterogeneous nucleation in the cirrus scheme, which increased ice crystal sizes, Gasparini et al. (2018) were able to reduce γ_{s} by an order of magnitude compared to the reference ECHAM-HAM version (Blaž Gasparini, personal communication, 2021). This in turn would be expected to reduce the importance of autoconversion in the present analysis. Moreover, the design choices of the CMP scheme, e.g., the order in which processes are called, may also influence the results. However, learning about the properties of CMP processes in the ECHAM-HAM model is important, no matter whether they are physically based or artificially introduced through model design.

A caveat to these results is of course that only CMP processes were investigated here. Parameters or processes from other parts of the climate model, e.g., the dynamics, might exhibit an even larger influence on the investigated model output if they were allowed to be varied. For example, Wellmann et al. (2020), using idealized COSMO simulations, found that environmental conditions are more influential for the diabatic heating rates than microphysical processes. However, for the research question at hand, namely how accurate the representation of these four processes within the CMPs needs to be, the comparison of the processes between each other is sufficient. Indeed, the negligible sensitivity of model output to variations in accretion and self-collection of ice suggests that their representation may be simplified (Lee et al., 2012). Due to the small deviations in the considered variables in response to variations around $\eta_i = 1$ for riming and autoconversion (purple line in Fig. 2.2), there is potential for simplifications of their formulations. In the grand scheme of CMP parameterization development, however, autoconversion as the most dominant process of the four is a key process to scrutinize given the possibly troubling origin of this dominance in its role as a tuning factor.

2.3.4 Scale dependency analysis

The analysis of global annual mean values yields clear conclusions, but climate models need to simulate not only global mean values correctly but also their spatial and temporal evolution. Since the emulation and subsequent analysis of grid-point-level data is tedious and error-prone due to the small signal and large noise, we compress the information in the data to a space of lower dimensionality. Choosing to reduce the dimensionality but still represent the whole global data rather than picking certain regions allows for a more objectified and unbiased analysis. This is similar to Holden et al. (2015), who also reduce their high-dimensionality output, albeit with singular value decomposition, and Ryan et al. (2018), who use principal component analysis. However, as the model data are complete and on a sphere, a spherical harmonics expansion is our method of choice.

Mathematically, the model data can be represented as a linear combination of the orthogonal spherical harmonics basis functions as follows:

$$f(\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} F_l^m Y_l^m(\theta,\phi). \tag{2.5}$$

The data represented by f are then a function of the longitude θ and latitude ϕ, with Y_l^m a spherical harmonics function of degree l and order m (l and m are integers, with $-l \leq m \leq l$). The complex coefficients F_l^m can be computed as

$$F_l^m = \int_\Omega f(\theta,\phi) Y_l^m(\theta,\phi) \mathrm{d}\Omega. \tag{2.6}$$

The coefficients make up the angular power spectrum S_{ff}:

$$S_{ff}(l) = \frac{1}{4\pi} \sum_{m=-l}^{l} |F_l^m|^2, \tag{2.7}$$

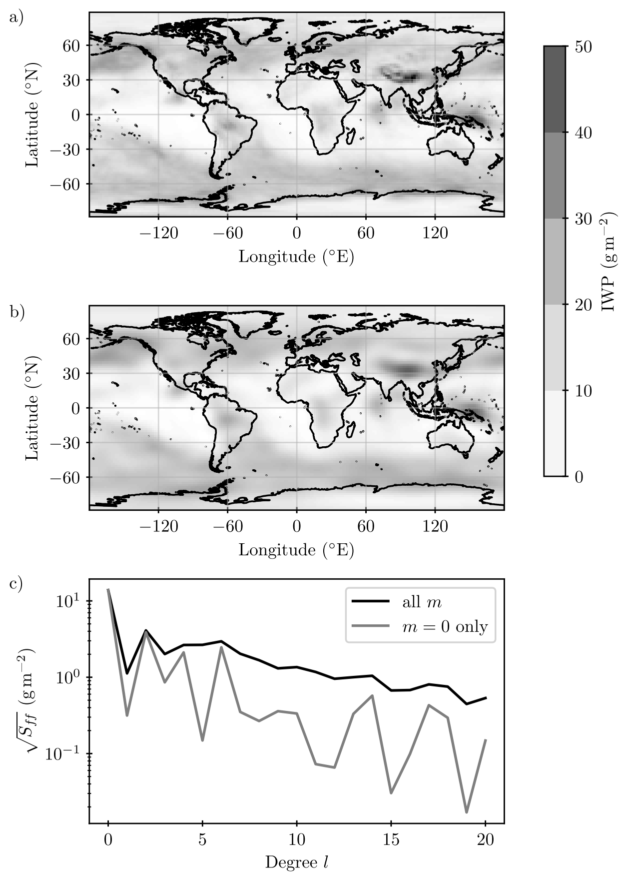

Figure 2.10: Spherical harmonics expansions for one illustrative PPE member ($\eta_{\text{autc}} \approx 0.87$, $\eta_{\text{accr}} \approx 1.43$, $\eta_{\text{rime}} \approx 0.81$, $\eta_{\text{sci}} \approx 1.89$). **(a)** Global annual mean IWP and **(b)** expansion of spherical harmonics representing the same data as **(a)**, generated from the coefficients of the expansion displayed as an angular amplitude spectrum in **(c)** as a function of the degree l (with m independent solutions, where modes of $m = 0$ most strongly resemble rotationally symmetric physical patterns of the Earth system such as a north–south contrast). Note that the variability explained by each degree l in general decreases with increasing l, which allows us to truncate the expansion at the degree l where it represents 95 % of the total data variance.

where the sum over the angular power spectrum $\sum_{l=0}^{\infty} S_{ff}(l)$ is the variance of the data. In principle, an expansion up to order 95 would represent the model data at their resolution of 96 latitudinal and 192 longitudinal points perfectly, as they are equidistant in spherical coordinates. In practice, we truncated the expansion at the degree l where it represents 95 % of the total data variance $\sum_{l=0}^{\infty} S_{ff}(l)$. Thereby we represent the data with as few as possible but as many as necessary basis functions. Note that in principle, a principal component analysis could yield the same representation with fewer basis functions. However, these functions would depend on the investigated dataset, while the use of spherical harmonics allows for intercomparability.

Figure 2.10 illustrates that a spherical harmonics expansion of the data can serve as an accurate representation, while all the information can be stored in the coefficients up to $l = 20$ instead of on the global grid (see Fig. 2.10c). Thus, confident that the expansion represents the data accurately, we can conduct a spatially resolved sensitivity analysis in the spherical harmonics space. For each variable and degree l a

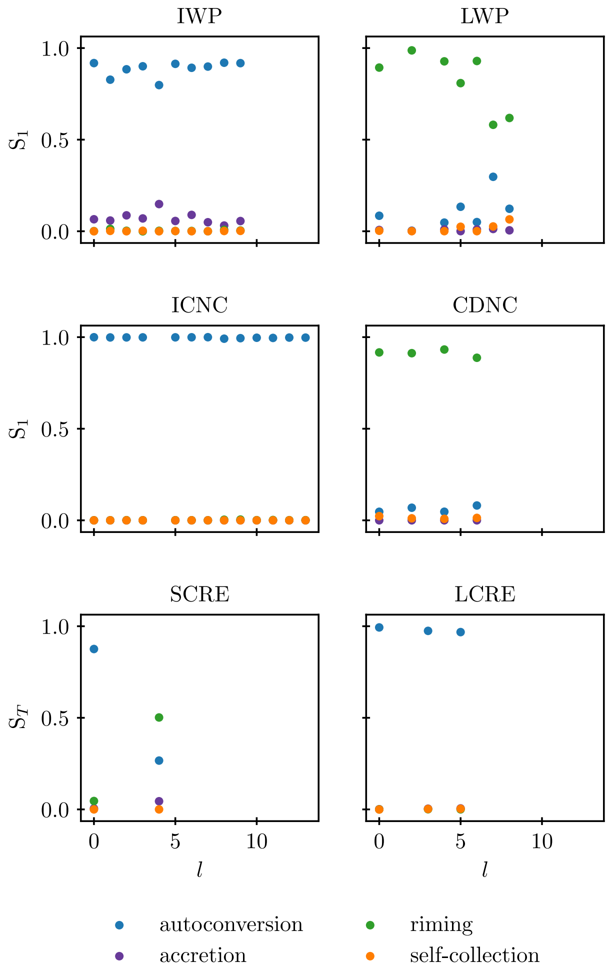

Figure 2.11: First-order sensitivity indices for the emulated angular amplitude spectrum as a function of the spherical harmonics degree l for the variables as described for Fig. 2.9. As detailed in the text, emulators that were found to be defaulting in the validation procedure were not subjected to the sensitivity analysis so that the results for those l are missing here. The results for the total sensitivity index are shown in Fig. A.2 in Appendix A.3.

separate emulator was trained on the angular amplitude spectrum $\sqrt{S_{ff}}$, from which samples were drawn as input to the sensitivity analysis. The validation procedure was the same as described in Sec. 2.2.4. Spherical harmonics members of degree l were excluded from the sensitivity analysis when the emulator was found to be defaulting to an equal prediction over the phase space (see Appendix A.4). This was the case mostly for degrees l for which the coefficients could already be seen to have less amplitude in the angular amplitude spectrum. A total of 5 out of 11 variables had to be excluded because too many members were defaulting or because their variations were too small to be sensibly emulated.

The results are displayed in Fig. 2.11. For those variables that had total sensitivity indices for autoconversion of over 0.9 (IWP, longwave cloud radiative effect, and ICNC) the dominant effect of autoconversion is present on all length scales. Accretion is of secondary importance for the IWP, as indicated by the global sensitivity analysis. The LWP and CDNC are dominated by riming on all regional scales and on the global scale.

The emulated surfaces for the spherical harmonics are more uncertain than those for the global mean values (see Appendix A.4). This is expected as the training data are more noisy and indicate a less detectable signal on smaller length scales than on the global one. In addition, the separate emulation for different degrees l ignores correlations between signals included in multiple degrees l, which may lead to the loss of signals that are small in the different l but correlated, and should therefore be addressed in future studies. However, as the results of the sensitivity analysis are clear in that variability is dominated by autoconversion (see Fig. 2.11), we can conclude that the results of the global sensitivity analysis also hold on regional scales.

Finally, this analysis demonstrates that spherical harmonics expansion is a viable tool to evaluate model output on all length scales in an efficient and objective manner. Future studies may use it to compare results, e.g., from different models. As most expansion degrees are physically difficult to interpret, the method may be expanded to use physically meaningful modes such as the land–sea contrast instead.

2.3.5 Seasonal analysis

Similar to a regional analysis, we use a temporally resolved sensitivity analysis to address the concern that conclusions drawn from annual mean values might not hold on a seasonal scale. Figure 2.12 shows the results of the same sensitivity analysis as in Fig. 2.9, but split by seasons (one emulator per variable was trained and validated for each season; note that in a few cases only 47 PPE members were used as with the 48th member the computational constraint was too tight for the emulator). Due to a weaker or less consistent signal in the data on seasonal scales, one variable (mixed-phase cloud cover in MAM) did not pass the validation procedure as the emulator was found to be defaulting (as described for the spherical harmonics above and in Appendix A.4). Figure 2.12 reveals that indeed the sensitivities to process perturbations are much the same as for the annual mean analysis. This confirms that the conclusions drawn for model simplifications also hold on a seasonal scale. The model is not sensitive to accretion and self-collection of ice, and therefore these processes can be simplified, while autoconversion and riming dominate the model response.

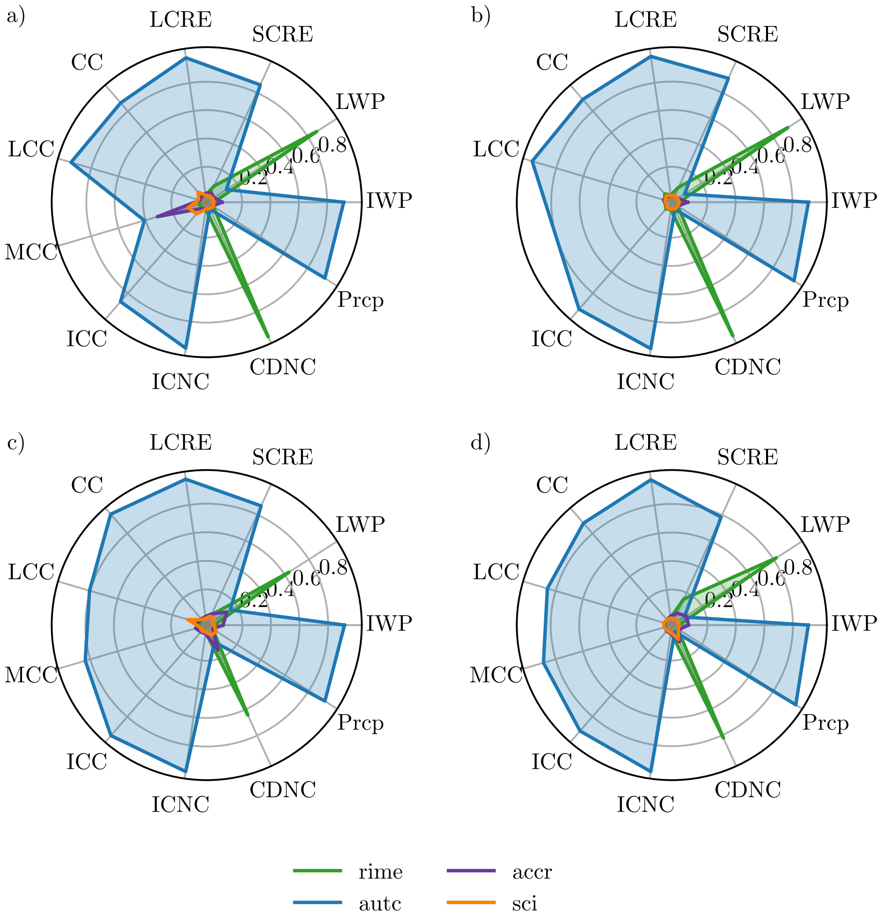

Figure 2.12: Same as Fig. 2.9 but with seasonal means (**a**: DJF, **b**: MAM, **c**: JJA, **d**: SON) and only first-order sensitivity indices shown. The results for the total sensitivity index are shown in Fig. A.3 in Appendix A.3.

Table 2.1: Share of the computing time taken up by the cloud microphysical processes investigated here. In turn, the CMP computing time represents 4.7 % of total computing time (excluding diagnostics; all values averaged over a 12-month control simulation with $\eta_i = 1 \forall i$). The time in the subroutine cold precipitation formation that is not attributed to the four processes is used for common initializations and subsequent processing.

Process	Share of CMP routine cost (%)
Riming	1.8
Autoconversion	0.62
Accretion	0.46
Self-collection	0.046
Subroutine cold precipitation formation	4.8

2.3.6 Process costs and implications for simplification

The previous analysis shows that the response of ECHAM-HAM to a suppression of self-collection or accretion is negligible, while for riming and autoconversion a less accurate representation may be appropriate. A potential benefit could lie in the reduction of CPU time per model simulation. Table 2.1 lists the CPU time spent in the CMP routines of the four processes. The timings represent an estimate of how much time could be gained by removing a process from the model. They show that, at most, with naively removing (the most drastic simplification) the whole cold precipitation formation routine, only about 0.2 % of total computing time can be saved (since the cold precipitation formation routine makes up 4.8 % of the 4.7 % of computing time that the whole CMPs take up, see Table 2.1). In a 10-year simulation this would allow for 1 additional week of simulation, which is negligible in comparison to the computing needs of, e.g., increases in model resolution.

Within the CMP routine there are other physical processes that take up time, but the calculations of diagnostics and preparatory calculations also contribute. Of course, if numerous CMP processes and interactions with aerosols were simplified, this would allow for more drastic steps such as fewer prognostic aerosol variables as those could become redundant. Subsequently, significant reductions in model cost could be achieved. Yet by itself, the isolated removal or simplification of CMP processes provides small leverage for a decrease in computing time. However, as detailed in Sec. 2.1, there are numerous benefits in simplification that are independent of the associated computing cost, such as a gain in compactness and interpretability.

2.4 Summary, conclusions and outlook

This study conducted a sensitivity analysis with an emulated PPE to illuminate the impact of selected CMP processes on model output. Different from previous studies (e.g., Wellmann et al. (2020) and Hawker et al. (2021b)), we perturb the four CMP processes of autoconversion, riming, accretion, and self-collection of ice as a whole. This is achieved by multiplying their process rates with a factor between 0.5 and 2. The resulting response surface of model output and its deviation from results with the default setup serve as a proxy for how accurately a process needs to be represented.

Perturbing only one process at a time reveals that ice crystal autoconversion acts as a threshold process: perturbing it causes the model to deviate, but when it is turned off the deviation is immense. This is because it is the only process that converts ice crystals to snow and as such accretion and riming depend on it. Using only roughly twice as many simulations as in the one-at-a-time perturbations to generate a PPE, we can generate the whole response surface using Gaussian process emulation. A sensitivity analysis of global and seasonal annual means reveals that for cloud cover, ice water path, and number concentration as well as shortwave and longwave radiative effect, the perturbation of autoconversion has the most dominant impact by far. Accretion and riming assume a secondary role. As riming is the only investigated process that directly affects the liquid phase, riming has a dominant effect on the liquid water path and cloud droplet number concentration. Self-collection of ice has a negligible impact on the investigated global annual mean variables. Resolving smaller horizontal scales using a spherical harmonics expansion of the output variables corroborates the results of the global annual mean analysis, as does a seasonal analysis. These results, as well as the shape of the response surface, suggest that the parameterization of self-collection and accretion can be readily and drastically simplified. While autoconversion and riming have a large impact on the model output considering the whole investigated phase space, the shallow slope of the response surface around the default $\eta_i = 1$ hints that slight modifications of their representations may leave the model output unchanged. The strength of the PPE approach is that interactions are already taken into account, meaning that all four processes could be simplified at the same time. If one wants to develop the CMP scheme further, autoconversion is the process to scrutinize as it has the largest leverage in the model and therefore the most urgent need to be represented correctly.

As we find that the processes themselves use a negligible fraction of the overall model computing time, simplifications are proposed as a means to make the model more interpretable, not cheaper (see Secs. 2.1 and 2.3.6). Our analysis shows that the representation of the four investigated microphysical processes leaves room for simplification. However, in deciding how drastic these simplifications should be, process uncertainty should also be considered. At the least, when new parameterizations are included in climate models we should also question their implementation regarding the complexity they add, looking for their consistency, interpretability, simplicity, and comprehensiveness (Mülmenstädt and Feingold, 2018; Touzé-Pfeiffer et al., 2021). Of course, more drastic simplifications than process reformulations would provide more leverage on interpretability and computing cost. For example, CMP schemes that contain only one category for ice, e.g., the predicted particle properties (P3) ice microphysics scheme (e.g., Morrison and Milbrandt (2015), Eidhammer et al. (2017), Dietlicher et al. (2018), Dietlicher et al. (2019), and Tully et al. (2021)) are more physical as well as more interpretable. From this perspective it might seem troubling that in the current CMP scheme the autoconversion process, which is a transfer mechanism between the two artificial classes, is so dominant in its importance. However, while the categories are artificial, the process itself is not: accretion of ice crystals forming larger ice crystals would be the equivalent process with only one ice category. Still, autoconversion is difficult to constrain in observations (Morrison et al., 2020) also because it is not a distinct physical process, so moving towards a scheme with evolving instead of pre-defined ice categories seems advisable (see, e.g., Milbrandt and Morrison (2016) and Jensen et al. (2017)).

This study introduces the methodological framework to study the sensitivity of a climate model to the representation of CMP processes. To complete it, the analysis needs to be expanded to include other CMP processes in the model: for cold CMP ice formation, regional modeling studies have demonstrated cloud susceptibility to the choice of the ice nucleation parameterization (Levkov et al., 1995a; Hawker et al., 2021b), whereas in ECHAM-HAM heterogeneous immersion freezing in mixed-phase clouds has been shown to be rather inefficient (Villanueva et al., 2021). More generally the heterogeneous ice formation pathway in mixed-phase clouds is small in ECHAM-HAM (Dietlicher et al., 2019; Bacer et al., 2021), hinting at simplification potential. In a sensitivity study of CMP parameters, Tan and Storelvmo (2016) found that the timescale of the Wegener–Bergeron–Findeisen process explains a large variance in supercooled cloud fractions, suggesting that as a whole it may be a dominating process as well. Secondary ice formation (Korolev and Leisner, 2020) may interact with the ice crystal source processes, allowing for interactive sensitivities (Hawker et al., 2021b), and should therefore be included, even though only the Hallett–Mossop process is optionally included in ECHAM-HAM (Neubauer et al., 2019). Moreover, for a complete CMP process investigation, of course the warm-rain processes need to be included as well (Wood et al., 2009; Gettelman et al., 2013).

One might argue that our analysis neglects the influence of other factors external to the CMPs on our conclusions. However, as our simulations span the whole globe and a whole year, they cover a range of dynamical situations, and the results are therefore robust in the current climate. Whether the conclusions hold, e.g., in a future changed climate will have to be evaluated in a future study. It is important to stress that while we propose that simplifications to the CMP representation are possible, care needs to be taken to leave them physically based to ensure that the model can correctly represent differing climates. We emphasize that our findings are conditional on the design of the ECHAM-HAM model, including the implementation of other processes and parameters that were not varied in the current study. Another factor that has not been investigated here is the model resolution that may affect the CMP behavior in the model and thereby our conclusions on the importance of single processes (Santos et al., 2021). The implementation and design choices of the CMP scheme in ECHAM-HAM may also influence the results, e.g., in the order of processes that are called, the separation between ice and snow, and the employed tuning strategy. Thus, the results as such are only applicable to this CMP scheme and cannot be transferred to the significance of the investigated processes in other schemes let alone in reality.

Nevertheless, learning about the representation of CMP processes in ECHAM-HAM and how sensitive the model is to their representation helps us to interpret and improve the model, especially when comparing the results to experimental studies. To this end, it will also be fruitful to compare our findings to sensitivities in other models using different CMP schemes.

Code and data availability The ECHAM-HAMMOZ model is freely available to the scientific community under the HAMMOZ Software License Agreement, which defines the conditions under which the model can be used. The specific version of the code used for this study is archived in the ECHAM-HAMMOZ SVN repository at /root/echam6-hammoz/tags/papers/2022/Proske_et_al_2022_ACP_2. More information can be found on the HAMMOZ website[1]. Analysis and plotting scripts are archived at https://doi.org/10.5281/zenodo.5506588 (Proske et al., 2022c). Generated data is archived at https://doi.org/10.5281/zenodo.5506533 (Proske et al., 2022b). The PyDOE library (tisimst, 2021) was used for Latin Hypercube Sampling, ESEm (Watson-Parris et al., 2021c; Watson-Parris et al., 2021a) for the construction of the emulator, SALib (Usher et al., 2020) for the sensitivity analysis, and PySphereX (Staab, 2021) for the construction of the spherical harmonics expansion.

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Throughout this study, the programming languages CDO (Schulzweida, 2018) and Python (Python Software Foundation, www.python.org) were used to handle data and analyse it. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 821205 (FORCeS).

[1] https://redmine.hammoz.ethz.ch/projects/hammoz, last access: 17 September 2021

3

Addressing complexity in global aerosol climate model cloud microphysics

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Abstract In a quest to represent the Earth system, climate models have become more and more complex. This generates problems, for example hindering model interpretability. This study contributes to a regain of model understanding and proposes simplifications to decrease scheme complexity. We reflect on the reasons for model complexity and the problems it generates or deepens, connecting perspectives from atmospheric science and the philosophy of climate science. Using an emulated perturbed parameter ensemble of the cloud microphysics (CMPs) process efficiencies, we investigate the sensitivity of the model to process perturbations. The sensitivity analysis characterizes the scheme and model behavior, contrasting it to physical process understanding as well as an alternative CMPs formulation (comparing the 2M (Lohmann et al., 2007) to the P3 scheme (Morrison and Milbrandt, 2015; Dietlicher et al., 2018)). For the 2M scheme, ice crystal autoconversion dominates the model sensitivity in the ice phase. The P3 scheme removes this artificial process and

thus shows more balanced sensitivities. Model behavior sometimes aligns with process understanding, but many process sensitivities are masked by other more dominant processes or the model finally responds differently due to adjustments. We identify processes that the model is not sensitive to and test their simplification. For example, heterogeneous freezing or secondary ice production are drastically simplifiable. Depending on one's modeling vision one may interpret this study's findings as pointing to simplification potential in the CMPs scheme or the need for process representation improvements where the model behavior does not tally with our physical understanding.

Plain Language Summary Climate models are supposed to help us to understand or project Earth system behavior. In order to represent many aspects of this system, modelers have added more and more detail to the models. This makes the models complex and difficult to understand, even for the modelers themselves. We want to gain more understanding of the model behavior. For this we use a methodology where we manipulate the effectiveness of a process in the model to test how the model reacts to that change. Some of how the model reacts is surprising and different from what our physical understanding of a process suggests. In particular, some processes, like the freezing of cloud droplets at temperatures warmer than $-35\,^{\circ}\mathrm{C}$, are negligible in the model, even though atmospheric scientists think that this is an important process in the real atmosphere. Now one could either simplify the representation of such a process, or try to improve the model to reflect physical reality better. What one decides for depends on the purpose and concept of the model.

3.1 Introduction

In climate modeling, our task is to represent an immensely complex system which we wish to understand and learn about. Model development inherently faces tradeoffs between epistemic values like tractability, interpretability, validation potential, and specificity (Larsen et al., 2016; Undorf et al., 2022; Beucler et al., 2021), which manifest themselves in the ever present question of where to draw the line for details. Understanding nature requires a simplification of the mechanisms at play, but wanting to be precise calls for more details that increase complexity (Tapiador et al., 2019). For the term "model complexity" we here follow the "loose definition" mentioned in García-Callejas and Araújo (2016) that a model becomes more complex the more difficult to comprehend its computations are and the more processes/computations there are (Randall et al., 2003; Baartman et al., 2020).

Climate modeling has followed the *mirror view* (Parker, 2022a), meaning that it wants to mirror the Earth system in the model representation. Different modeling approaches would be following for example the predictive or heuristic view, which aim for predictive abilities or the ability to generate understanding, respectively; see for example Held (2005), Lahsen (2005), Sundberg (2009), and Heymann and Hundebol (2017). In particular, deducing representation from detailed first-principles is favored in geological modeling (Larsen et al., 2016). Following the mirror view, improving climate models means trying to represent the system better and this is achieved by adding more and more detail and hence the models have grown more complex (Edwards, 2011; Stevens and Bony, 2013). In the face of complexity and uncertainty, more detailed or physical formalisms are an anchor to hold onto; but sometimes it also seems like this quest for more detail is merely the capitulation in front of a complex system that we cannot grasp otherwise (Saltelli et al., 2020b). The complexity in process representation brings about a bouquet of problems for the model:

1. **Hindered understanding** Too many detailed processes hinder the modeler's understanding of the model (Menard et al., 2021). Many of these processes have been added in the first place to test their impact, and may only stay included to reassure that nothing that might be of importance is left out, meaning that the model is used as a book-keeper. However, having more and more processes included does not improve interpretability of the model. Gramelsberger et al. (2020) have termed this the "dilemma of growth": models are meant to aid understanding of something as complex as the Earth system, but "the growing complexity of the models themselves seems to jeopardize understanding" (see also Held (2005)). As the model is built up sequentially, every added process deepens the *generative entrenchment* (meaning an entanglement in climate model evolution with development steps depending on each other so that modeling options depend on previous choices (Lenhard and Winsberg (2010) adopting a concept introduced by Wimsatt (2007) for climate science); also termed path dependence or legacy effect by Babel (2019)).

2. **Equifinality** More processes mean more free parameters, which need to be set via tuning and may allow for multiple equally plausible model realizations with similar or indistinguishable results (Beven and Freer, 2001; Beven, 2006; Tapiador et al., 2019; Mülmenstädt et al., 2020).

3. **Overinterpretation** Including more processes or more sophisticated schemes brings the danger of overinterpreting the processes that are represented while neglecting the impact of "minor-looking treatments" such as thresholds (Kawai et al., 2022) or of those processes that are not represented (Mülmenstädt and Feingold, 2018). Provocatively put, the research into and representation of more and more processes may even be acting as an "engine of distraction," meaning that it may obscure elemental relationships or other study objects and that thus the detail produces ignorance (Proctor and Schiebinger (2008) citing Wes Jackson for the term on p. 24).

4. **No reduction in uncertainty** At the same time, the increase in model and process complexity may not be decreasing uncertainty (Lahsen, 2005; Mauritsen et al., 2012; Knutti and Sedláček, 2013; Stevens and Bony, 2013; Carslaw et al., 2018; Fiedler et al., 2019b; Puy et al., 2022), increasing the abilities of the model (see e.g., Zelinka et al. (2022) for the representation of clouds in improving cloud feedback representations; Krinner et al. (2018) and Menard et al. (2021) for a snow model intercomparison; Crout et al. (2009) for different environmental models) or the confidence in its results. Baartman et al. (2020) have surveyed geoscientists' opinions on model complexity. Respondents disagreed strongly that models will be improved by making them more complex. In particular, more experienced modelers are more cautious/suspicious of complexity and disagree that a more complex model warrants more confidence than a simple one.

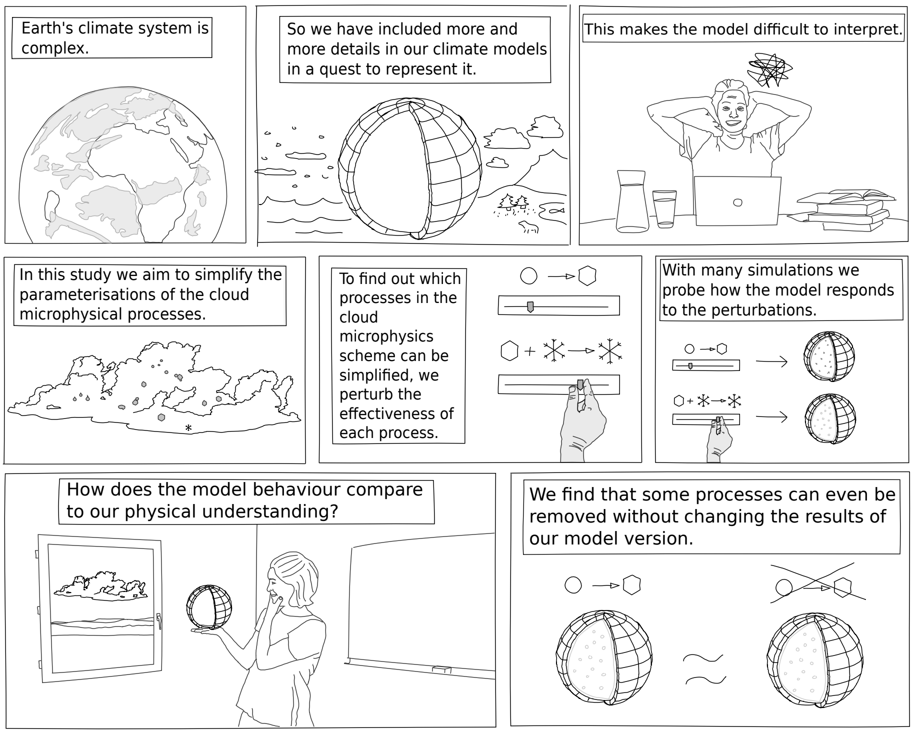

Figure 3.1: Visualization of the motivation and methods in this study.

5. **Hides non-epistemic influences** The opacity (Undorf et al., 2022) and the authority (Heymann et al., 2017b) of the global climate model hide above methodological problems. They also conceal the influence of non-epistemic values (Pulkkinen et al., 2022) and habits (Babel, 2019) involved in model construction. Especially the influence of the modelers' unforced choices makes it even more important to scrutinize what has been included (Winsberg, 2012; Ward, 2021). Non-epistemic values refer to those values that do not contribute "to the goal of gaining knowledge," such as moral or political values (Elliott, 2017; Undorf et al., 2022).

In summary, as Guthke (2017) argues, complexity needs to be tailored to the model's purpose (Parker, 2020).

Thus, it may well be time to scrutinize the complexity that has accumulated, characterize the current model schemes, evaluate which processes have a significant effect on global model results (within the framework of our scientific questions cloud properties are especially relevant) and simplify or remove the ones that do not. In this study, we are documenting and characterizing the 2-moment cloud microphysics (CMPs) scheme and are comparing it to the P3 CMPs scheme as well as physical understanding (see Fig. 3.1). Previous studies have used different methodologies to understand model behavior, for example Dietlicher et al. (2019) have introduced a pathway analysis of ice formation or Bacer et al. (2021) have analyzed the process rates of cloud microphysical (CMP) processes in ECHAM-HAM. However, to our knowledge we present the first sensitivity analysis encompassing the whole CMPs scheme and the resulting global variables. Then we metaphorically put on Ockham's razor, asking what can be left out of the CMPs in a global climate model, with the model staying equifinal (Beven and Freer, 2001; Beven, 2006). Instead of the mirror view we aim for *adequacy for purpose* (Parker, 2020). If the purpose of the model is explanatory, even more accurate but complex equations make it less adequate for purpose. Instead, simplicity aids understanding, and thus reducing the amount or complexity of process representations serves the models' adequacy. Another model purpose could be predictive accuracy, where processes that the model is not sensitive to do not increase the model's adequacy. Note that the focus of our study is explicitly on enhancing interpretability of the model and not on computational time savings. One might expect simplifications to serve reductions in computational cost, but Proske et al. (2022a) have shown that the contributions of single CMP process computations to ECHAM-HAM simulation time are negligible (see their Table 1).

Simplifications of aerosol and climate models have been successfully attempted (Molteni, 2003; Ghan et al., 2012), for example for the representation of the aerosol radiative effects with a plume model (Stevens et al., 2017). Conversely, there are also studies that implement more detail into parameterizations and find small effects. For example, Karset et al. (2020) have added a size dependence to the parameterization of entrainment and evaporation and find a small impact on the radiative forcing due to aerosol-cloud interactions.

Also, the authors acknowledge that there are numerous other paths being advocated and followed to address the issue of complex climate models. Replacing climate models with emulators or other machine-learning generated surrogates is an emerging yet contested field (e.g., Knüsel (2020), Rudin (2019), Kasim et al. (2020), Nonnenmacher and Greenberg (2021), Beusch et al. (2022), and Watson-Parris et al. (2022)). On a smaller scale, machine-learning is also used to replace or improve single parameterizations or schemes (e.g., Seifert and Rasp (2020), Gettelman et al. (2021), Harder et al. (2021), and Meyer et al. (2022)). However, while these approaches may help to reduce the computational load of climate simulations, they do little to improve interpretability of the model (Rudin, 2019). Another approach follows the idea that in order to simulate climate, many of the details at finer scales are irrelevant to be forecasted explicitly and can thus be incorporated in stochastic models that make use of statistical laws at the macroweather time scale (see e.g., the fractional energy balance equation FEBE (Procyk et al., 2022; Lovejoy, 2022)). Similarly, Palmer (2001) questions the use of deterministic parameterizations and suggests to incorporate the variability on scales smaller than the model resolution stochastically. In our analysis, we stay with the classical, theory- or observation-based parameterizations as they summarize physical knowledge and establish the climate model's ability to simulate past and possible future climates (Couvreux et al., 2021). Here we study the model as it is and therefore look for simplification potential inside the established structures. To the authors' knowledge there have been no systematic attempts to reduce the number of processes or their level of detail in a whole model scheme while leaving the scheme structure itself intact. Here we attempt such a thorough but minimally invasive investigation for the CMPs scheme in the global climate model ECHAM-HAM.

The focus of the current analysis is the CMPs, which means all processes and hydrometeor interactions taking place inside clouds, representing a chaotic but buffered system (Tapiador et al., 2019). Clouds themselves are an integral part of the climate system, influencing the Earth's radiative and hydrological balance. This influence is in turn mediated by the clouds' microphysical properties, which thereby modulate important yet uncertain climate feedbacks and aerosol cloud interactions (e.g., Boucher et al. (2013) and Gettelman (2015)). Importantly, while the need for convection parameterizations will disappear with the move to higher resolution modeling, CMPs will continue to need to be parameterized at any resolution above the molecular scale (Morrison et al., 2020) (following the traditional rather than the statistical modeling approach mentioned above). Thus, the question of where one can draw the line for detail in CMPs is of lasting importance.

In climate models, CMPs are parameterized in different ways, from bulk to bin schemes, with one- (mass concentrations) or two-moments (mass and number concentrations) for the hydrometeors. These parameterizations are a good example of detailed schemes that are becoming problematic for interpretation as discussed above. In particular the CMPs scheme in ECHAM-HAM has a long history of additive development (see e.g. Lohmann and Roeckner (1996), Lohmann et al. (1999), Lohmann and Kärcher (2002), Hoose et al. (2008b), Joos et al. (2008), Lohmann (2008), Croft et al. (2009), Sesartic et al. (2012), Kuebbeler et al. (2014), Dietlicher et al. (2018), Friebel et al. (2019), and Muench and Lohmann (2020)), which deepens its generative entrenchment, while at the same time lacking clear documentation to aid interpretation. Randall et al. (2003) state that "the cloud parameterization problem is overwhelmingly complicated," and is becoming more so, because both numerical and conceptual complexity are rapidly increasing. The development of CMPs parameterizations may even be ahead of fundamental research (Morrison et al., 2020), as Hoose (2022) states for the process of secondary ice production. This may be for example, because the need to improve climate models is often employed as a justifying value (Ward, 2021) that encourages experimentalists to frame their research as contributing to parameterization development (Sundberg, 2007). Thus, with parameterizations that may not be grounded in thorough empirical or theoretical research, the CMPs scheme lends itself to simplification.

Practically, in the 2M scheme, the divide between ice crystals and snow flakes was modeled in analogy to the divide between cloud droplets and raindrops, which was based on sedimentation velocity (Lohmann and Roeckner, 1996). For the liquid phase, this divide into in-cloud cloud droplets and sedimenting raindrops is sensible, because there is a large gap in the fall speed of cloud droplets and raindrops. However, there is no such well-defined gap between ice crystals and snow flakes. Hence, the separation into a sedimenting snow and an in-cloud (not sedimenting) ice class is somewhat artificial for the ice categories. Subsequently, some of the connecting processes have artificial qualities in that they transfer between these two classes, even though they exist as real processes in the atmosphere (e.g., ice crystals really collide and form a larger ice crystal, but this resulting particle is termed a snowflake artificially in the process of ice crystal autoconversion in the model). To overcome the ill-constrained divide between ice crystals and snowflakes, schemes that represent ice as a single category with variable properties have been proposed. In particular, Morrison and Milbrandt (2015) have developed the P3 scheme that Dietlicher et al. (2018) have implemented into the ECHAM-HAM model. The P3 scheme has been evaluated as both producing results closer to observations and being more physical in the sense of closer to first principles (based on the absence of the artificial separation of snow categories) (Dietlicher et al., 2018; Wang et al., 2021). Hence Igel et al. (2022) call for such a single category in the liquid phase as well. We include the P3 scheme in our analysis here to broaden the scope to a more general treatment of CMPs schemes with differing properties.

To probe how ECHAM-HAM reacts to alterations of the CMPs scheme parameterizations, we employ extended sensitivity studies. In particular, we construct a perturbed parameter ensemble (PPE) of altered process efficiencies. We emulate the resulting response surface with a Gaussian Process emulator (Rasmussen and Williams, 2006; Watson-Parris et al., 2021b) to be able to conduct quantitative sensitivity analysis (Saltelli, 2008a). In this approach we follow Proske et al. (2022a), but extend their analysis to 15 CMP processes and the P3 scheme. The method of exploring a parameter space with a PPE has been employed widely in atmospheric science (Lee et al., 2011; Yan et al., 2015; Couvreux et al., 2021; Hawker et al., 2021a), but we direct it toward a new research question: we want to characterize the whole entangled system of CMPs parameterizations and use the results to determine which processes are negligible or can be simplified, aiming to reduce complexity. For simplifications we try removing a process and replacing its formulation by a constant (0 dimensional) or a zonal mean (2 dimensional) climatology. If a process is simplifiable without much effect on the model output, that either means it is negligible or points to something that is wrong in the model. As the climate model's key ability to simulate both past and possible future climates needs to be preserved for it to remain adequate for purpose, we test the performance of the simplifications we develop in different climate states.

3.2 Methods

As the present study is a continuation of the work in Proske et al. (2022a), the use of ECHAM-HAM, the construction of the PPE, the emulation and sensitivity analysis are akin. Thus we refer the reader to Proske et al. (2022a) for a detailed documentation of these methods, and in the following we provide only a brief overview.

3.2.1 Cloud microphysics in ECHAM-HAM

This study employs the aerosol-climate model ECHAM6.3-HAM2.3 (Tegen et al., 2019; Neubauer et al., 2019). It has 47 vertical levels and a T63 horizontal spectral resolution ($1.875^{\circ} \times 1.875^{\circ}$). Apart from additional perturbation parameters that we added (see Sec. 3.2.1), the model version used in this study is the same as in Proske et al. (2022a). The changes with regard to the published model version ECHAM6.3-HAM2.3 (Neubauer et al., 2019) as well as the tuning are thus documented in Proske et al. (2022a).

For stratiform clouds the default model version employs a 2-moment CMPs scheme that is visualized in Fig. 3.2. Cloud droplets and ice crystals are treated prognostically in both mass and number concentrations (the first two moments of a distribution). Snow and rain are diagnosed and reach the surface within one timestep but undergo processes and transformations while sedimenting through the model levels. The four hydrometeors interact with each other and with water vapor through linear and non-linear processes. For example, the sublimation of snow forms water vapor, or two ice crystals form one snowflake in the process of ice crystal autoconversion.

Some of the process formulations are simple. For example, in-cloud melting occurs at temperatures above 273.15 K and transforms all ice crystals into cloud droplets. Because these physical and simple formulations offer no potential for a simplification, they are excluded from the following analysis (marked gray in Fig.

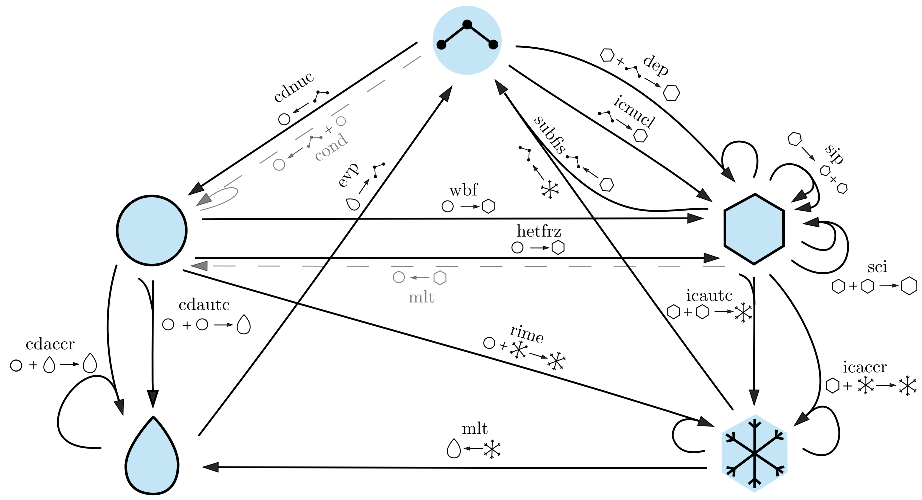

Figure 3.2: Schematic of the cloud microphysical processes included in the ECHAM-HAM 2-moment cloud microphysics scheme, connecting water vapor (top), cloud droplets (top left), rain drops (bottom left), ice crystals (top right), and snowflakes (bottom right). Processes that are present in the scheme but not part of the present analysis are represented in gray. Acronyms for the processes are explained in Table 3.1.

3.2). Other process parameterizations are sophisticated. For example, sublimation takes into account the saturation vapor pressure, the ventilation effect as well as the latent heat release in a semi-empirical formula. Their complexity and specificity in the face of limited evidence to constrain them begs the question whether their formulation could be simplified. Thus, these processes are included in the following sensitivity study (marked black in Fig. 3.2). The CMP process parameterizations are detailed in Table 3.1 (for a comparison to CMPs schemes employed in other models see Tapiador et al. (2019, Table 2)). Documentation of the scheme in the literature and also within the model code is incremental and incomplete, as it is common for complex climate models (Winsberg, 2012; Menard et al., 2021). Summarizing the documentation of a module like this aims to ease understanding and reproducibility and to avoid mistakes as suggested by Menard et al. (2021).

The model treats convective clouds separately, except that their condensate can produce new stratiform clouds or thicken existing ones by convective detrainment. This study focusses on the stratiform cloud scheme.

Table 3.1: Origin of the cloud microphysics (CMPs) parameterizations in the 2M and P3 CMPs scheme. The acronyms from Fig. 3.2 that are explained here are printed in bold. Where they aid understanding, maximal and minimal conditions are made explicit. $f_{\mathrm{mlt},\Delta T}$ is the melted flux per temperature difference that the melting causes; $T_0 = 273.15\,\mathrm{K}$; F is the snow or ice flux in $\mathrm{kg\,m^{-2}\,s^{-1}}$; q_i is the mass mixing ratio of ice crystals $\mathrm{kg\,kg^{-1}}$; $f_{\mathrm{s,i}}$ is the ventilation factor of snow/ice; $E_{\mathrm{c,s/i}}$ is the collection efficiency between snow/ice and cloud droplets; ICNC abbreviates the ice crystal number concentration; α_i is a short-hand for terms involving multiple constants and variables, introduced to aid accessibility of the formulas.

Process Process	2M parameterization	2M reference	P3 parameterization	P3 reference
Melting **mlt**	Melting of sedimenting snow and ice: $F_{\mathrm{mlt,s/i}} = \mathrm{MIN}\left(F_{\mathrm{s/i}}, f_{\mathrm{mlt},\Delta T} \cdot (T - T_0)\right)$	Roeckner et al. (1992) and Lohmann and Roeckner (1996), but with a threshold of 273.15 K and not 275.15 K[1]	Melting of ice: $\frac{\partial q_\mathrm{i}}{\partial t} = \frac{\partial q_\mathrm{i}}{\partial t}_{\text{condensation}} + \frac{\partial q_\mathrm{i}}{\partial t}_{\text{diffusion}}$	Straka (2009, Equation 11.6) and Dietlicher et al. (2018, Equation 16)
Melting	Melting of in-cloud ice: $q_{\mathrm{mlt,i}} = q_\mathrm{i}$, where $T > T_0$, with $T_0 = 273.15\,\mathrm{K}$	Lohmann and Roeckner (1996)		

[1]In sensitivity tests, using one or the other temperature as T_0 made only a small difference (not shown).

Sublimation **subfis**	Sublimation of falling snow and ice: $F_{\mathrm{sub,s/i}} = \mathrm{MIN}\left(q_{\mathrm{sat,i}} - q, F_{\mathrm{sub,s/i}}\left(S_i, T, f_{\mathrm{s,i}}\right)\right)$	Lin et al. (1983, Equation 31), based on Byers (1965, Equation 5.29) (differs from Lohmann and Roeckner (1996), which is based on Roeckner et al. (1992) and does not take e.g. the ventilation effect into account)	Sublimation of ice: $\frac{\partial q_{\mathrm{i}}}{\partial t} = \mathrm{MIN}\left(\frac{\partial q_{\mathrm{i}}}{\partial t}_{\mathrm{deposition}}, 0\right)$, limited to ice saturation	Lohmann et al. (2016, Equation 8.11)
Evaporation **evp**	Evaporation of rain: $F_{\mathrm{evp,r}} = \mathrm{MIN}\left(q_{\mathrm{sat,w}} - q, F_{\mathrm{evp,r}}\left(S_{\mathrm{w}}, T, F_{\mathrm{rain}}\right)\right)$	Rotstayn (1997, Equation 23) (differs from Lohmann and Roeckner (1996), which is based solely on the saturation deficit (Roeckner et al., 1992))	Same as 2M	
Sedimentation	Sedimentation of ice: vertical advection, computing the fall speed Sedimentation of snow		Vertical advection, fall speed read from lookup table; requires temporal substepping	

Cloud droplet nucleation **cdnuc**	Köhler theory based	Abdul-Razzak and Ghan (2000)	Same as 2M	
Condensation	Saturation adjustment	Lohmann and Roeckner (1996)	Saturation adjustment	Dietlicher et al. (2018)
Deposition	Saturation adjustment	Lohmann and Roeckner (1996)	Saturation adjustment	Dietlicher et al. (2018)
Deposition **dep**	Deposition in cirrus clouds, solving the depositional growth equation	Kärcher and Lohmann (2002a)	Deposition in cirrus clouds: $\frac{\partial q_{\mathrm{i}}}{\partial t} = \mathrm{MAX}\left(\frac{\partial q_{\mathrm{i}}}{\partial t}_{\mathrm{deposition}}\left(RH_{\mathrm{i},C,T}\right),0\right)$	Lohmann et al. (2016, Equation 8.11)
Homogeneous freezing	All cloud droplets freeze at $T < T_0$		Semi-empirical homogeneous freezing rate	Jeffery and Austin (1997)
Heterogeneous freezing **hetfrz**	Immersion and contact freezing	Lohmann and Diehl (2006)	Same as 2M	
Ice nucleation **icnucl**	Nucleation of solution droplets in the cirrus regime	Kärcher and Lohmann (2002b) and Kärcher and Lohmann (2002a)	Same as 2M	
Autoconversion of CDs **cdautc**	$\left(\frac{\partial q_r}{\partial t}\right)_{\mathrm{cdautc}} = 1350 q_c^{2.47} N_c^{-1.79}$	Khairoutdinov and Kogan (2000, Equation 29)	Same as 2M	
Accrection of CDs **cdaccr**	$\left(\frac{\partial q_r}{\partial t}\right)_{\mathrm{cdaccr}} = 3.7 q_c q_r$	Khairoutdinov and Kogan (2000, Equation 34)		Same as 2M

Autoconversion of ICs **icautc**		–		
Accretion of ICs **icaccr**	As riming, but with $E_{\mathrm{s,i}} = e^{0.09(T-T_0)}$	Seifert and Beheng (2006, Equation 67)	–	
Self-collection of ICs **sci**	$\left(\frac{\partial \mathrm{ICNC}}{\partial t}\right)_{\mathrm{sci}} = \alpha_3 \mathrm{ICNC} \cdot q_i$		Analogous to riming	
Riming **rime**	$\left(\frac{\partial q_r}{\partial t}\right)_{\mathrm{rime}} = E_{\mathrm{c,s}} \alpha_4 q_l \left(\frac{1.3}{\rho_{\mathrm{air}}}\right)^{\frac{1}{2}}$	Lohmann (2004, Equation 1)	$\left(\frac{\partial q_r}{\partial t}\right)_{\mathrm{rime}} = \alpha_5 \cdot K \cdot E_{\mathrm{c,i}} \cdot \mathrm{ICNC} \cdot q_c \cdot \rho_{\mathrm{air}}$	Milbrandt and Morrison (2016)
Wegener-Bergeron-Findeisen process **wbf**	Threshold process: all droplets evaporate and deposit water onto existing ice crystals	Lohmann et al. (2007)	Extended saturation adjustment	Dietlicher et al. (2018)
Secondary ice production **sip**	$\left(\frac{\partial q_r}{\partial t}\right)_{\mathrm{sip}} = \alpha_6 E_{\mathrm{c,s}} q_c$	Lohmann (2002, p. 11) and Levkov et al. (1992)	–	

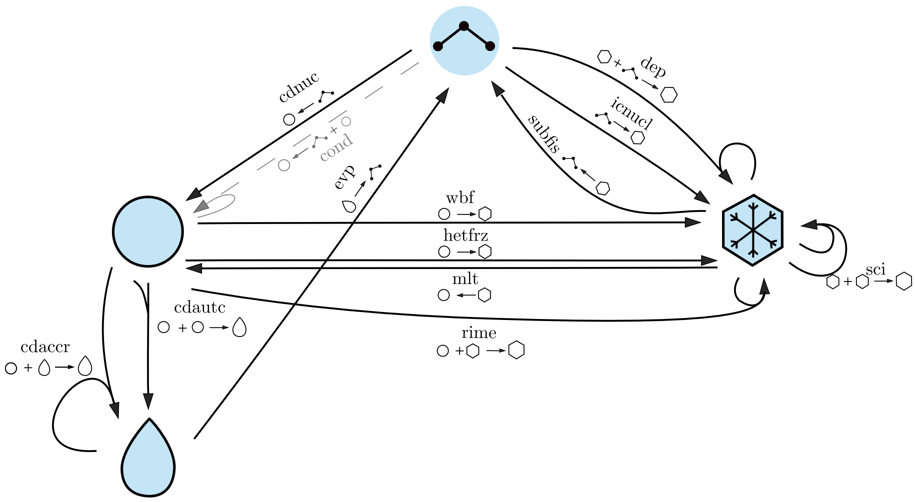

Figure 3.3: As Fig. 3.2 but for the P3 scheme.

P3 scheme

Dietlicher et al. (2018) have implemented the P3 CMPs scheme from Morrison and Milbrandt (2015) into the ECHAM6-HAM2 (echam6.3.0-ham2.3-moz1.0) (Zhang et al., 2012; Stevens et al., 2013) model. We have ported the scheme to the ECHAM6.3-HAM2.3 model version described above, including various bugfixes that have been developed in the meantime. This model combination is employed at the same vertical resolution of 47 levels in this paper (as the 2M model version) and required retuning that is detailed in Appendix B.1. The P3 CMPs scheme is visualized in Fig. 3.3 and the represented processes are detailed in Table 3.1. The scheme also splits the hydrometeors by size and assigns them different properties, such as the values for the ventilation coefficient at a given fall speed. However, they all participate in the same processes, for example snow and ice crystals are both sedimenting, so their artificial separation as in the 2M scheme is overcome (but a tuning factor for the aggregation of ice crystals, which corresponds to self-collection in the 2M scheme, remains). Another difference to the 2M CMPs scheme is that the P3 scheme introduces sub-time stepping to resolve the vertical advection of cloud ice and parallel splitting of the whole CMPs scheme (Dietlicher et al., 2018). This means that the CMP processes act on the same state of variables, whereas the 2M scheme employs sequential splitting, where processes are ordered and use the state updated from the preceding processes (Williamson, 2002; Zarzycki, 2022).

Perturbations

As introduced in Proske et al. (2022a) we use perturbations of the efficiency of single processes as a proxy for evaluating the model sensitivity to this process. If the model is sensitive to perturbations in a process, this suggests that this processes' representation is important and should be implemented accurately. However, if the model is insensitive to such perturbations, this suggests that the formulation of this process is not important and can thus be simplified. The perturbations are realised simply by multiplying the impact that each process i has on the CMPs variables by a factor η_i between 0.5 and 2 and are constant in time and space. The range is multiplicatively equally large on both sides of the default 1 (no perturbation), to sample over- and underestimations equally. A factor of 2 is deemed sufficient to approximate the effect of rough simplifications, but we note that this choice is underdetermined. If estimates for for example, the uncertainty of process formulations were available, this ad-hoc range could be replaced by a more physically meaningful one that could vary for each process. As estimating such a range would rely on a host of assumptions and unforced choices, we opt for equal ranges for all parameters. As detailed above, some process representations are so physical and simple that they were not perturbed here (e.g., melting). Some processes required implementation of condition checks after their perturbations to make sure that these do not push the model out of physically realistic conditions by for example, creating negative hydrometeor concentrations. These conditions may limit the sensitivity of the model to a given process. In particular, for the Wegener-Bergeron-Findeisen process the physical constraint renders efficiencies larger than 1 useless, because that would mean that more water droplets evaporate than are present.

3.2.2 Perturbed parameter ensemble, emulation, sensitivity analysis

In order to judge the effect of each process while taking into account interactions between processes, perturbations are applied to all processes at once in each simulation, thus creating a PPE. This experimental setup is visualized in Fig. 3.4. Expanding upon Proske et al. (2022a), who perturbed only four processes (self-collection and autoconversion of ice crystals, accretion of ice crystals with snowflakes, and riming), we are perturbing an additional 11 processes (see Table 3.1). The parameter space is sampled logarithmically because the perturbation parameters are multiplicative. To sample the space equally, we employ Latin Hypercube Sampling (Morris and Mitchell, 1995) as in Lee et al. (2011) and Hawker et al. (2021a). We choose 108 experiments, which is smaller than the 10 members suggested by Loeppky et al. (2009), but this criterion can be relaxed the more dimensions are added. For each of the PPE members, the full, global ECHAM-HAM model was run with the respective parameter combinations. These present day (PD) simulations were conducted for the year 2003, with a 3 months spin-up, climatological sea surface temperatures (SSTs) and sea ice extents, and aerosol emissions representative for the year 2003.

In order to be able to analyse the PPE results quantitatively, the results in the 15 process-dimensional parameter space were emulated. Gaussian process emulation was employed to model the behavior of each global annual mean variable of interest (one for each of the eight variables separately, namely ice crystal and cloud droplet number concentration (CDNC), ice and liquid water path (LWP), longwave and shortwave cloud radiative effect, cloud cover (CC) and precipitation). The emulation was conducted as described in Proske et al. (2022a).

Validation and sensitivity analysis

Validation of the emulator was conducted for each variable included in the analysis and conducted following Bastos and O'Hagan (2009) and as detailed in Proske et al. (2022a). It was performed as leave-one-out validation, where iteratively the emulator is trained on all experiments except one and its prediction is compared to the real simulated value. Fig. 3.5 displays the validation of the ice water path

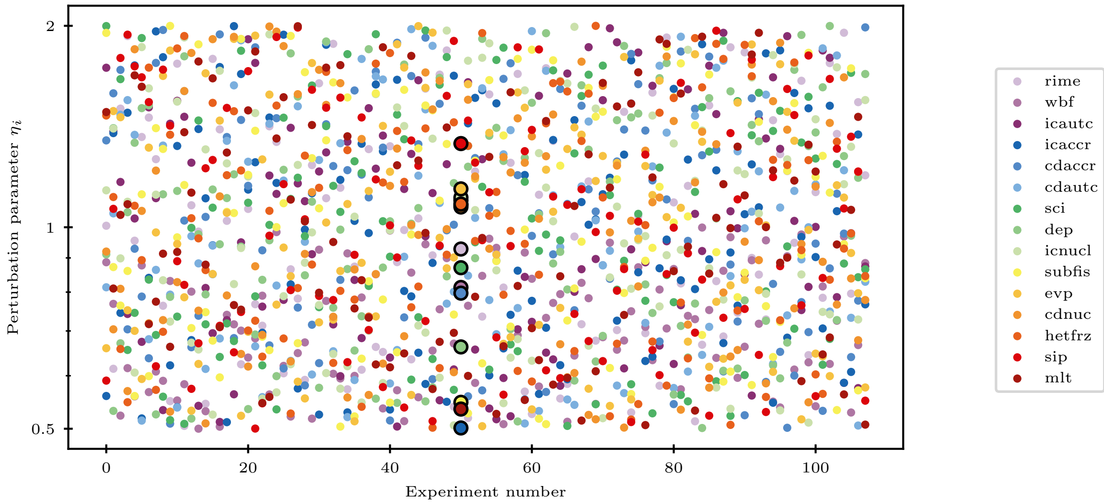

Figure 3.4: Perturbed parameter ensemble experimental setup. For each experiment (single vertical columns), the perturbation parameters of all processes were varied at once. Experiment number 50 is highlighted with black edges to illustrate this. The process acronyms are explained in Fig. 3.2 and Table 3.1.

(IWP) emulator. In Figures 3.5a and b we observe only few individual standardized errors larger than 2, which would signal a conflict. Fig. 3.5c indicates that the normality assumption used in a Gaussian process holds. In Fig. 3.5d, the actual values of emulator and real model output are compared. Points should lie close to the line of equifinality, with the 95% confidence bounds encompassing it. For IWP this is the case for 4 %, and for all variables this value lies between 2 % and 17 %. As there is good qualitative agreement between the emulator and real model output, no systematic bias exists. As we are looking for a conceptual analysis in this study, we deem the emulator representation of the model output to be sufficient.

Subsequently, variance-based global sensitivity analysis (Oakley and O'Hagan, 2004) was conducted on 3.000 points sampled from the emulated response surfaces to give quantitative estimates of the first order (S_1) and total sensitivity index (S_T) (as in Proske et al. (2022a)). S_1 of η_i measures the contribution of variance in η_i to the variance in an output variable such as IWP. S_1 lies between 0 and 1, where high values signal an important variable. S_T of η_i summarizes all direct and interactive effects that this parameter's variance has on the output variance (Homma and Saltelli, 1996; Saltelli, 2008b). Thus S_1 and S_T allow to determine the direct and the sum of direct and indirect effects of each process, respectively (Saltelli, 2008a).

Note that we use the emulation merely as a tool for model analysis. Our aim is by no means to replace model components with machine learned substitutes or to replace the full model (in contrast to e.g., Arcomano et al. (2022), Harder et al. (2021), and Fletcher et al. (2021)), but rather to understand how the model can be simplified.

3.2.3 Simplifications

Upon identifying processes to which the global model is insensitive, various forms of simplifications were tested. In order of severity or naivety, we tested removing a process, that is, setting the effect it has on model variables to zero; replacing

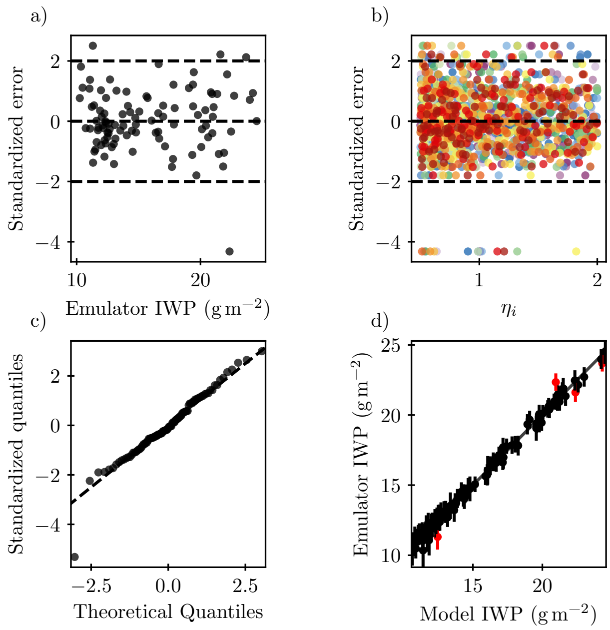

Figure 3.5: Leave-one-out validation of the emulator for the response of the global annual mean ice water path (IWP) in response to perturbations of the 15 processes, following Bastos and O'Hagan (2009) (same as Fig. 4 in Proske et al. (2022a)). Individual standardized errors are plotted against **(a)** emulator output and **(b)** input parameters (plotted separately for each process, colored according to Fig. 3.4). The standardized errors are computed as the difference between the real and emulated model output for IWP, normalized by the square root of V, the emulator variance: $\frac{\text{Model IWP}-\text{Emulator IWP)}}{\sqrt{V}}$. The dashed lines are drawn at an individual standardized error of 0 and 2, which is the threshold discussed in Bastos and O'Hagan (2009). **(c)** QQ-plot of the individual standardized errors against a student-T distribution. **(d)** Emulator against model output, with the error bars indicating the 95% confidence interval on the emulator predictions. Predictions for which the model result lies outside that interval are marked red.

the computed effect in the model with one constant for all grid points and times that the process is called; or replacing the effect with a constant climatology. This climatology was derived from monthly mean output of the process effect in a previous default simulation, with all η_i set to 1. As these values did not vary substantially in time and meridionally, we employed a zonal mean, but height resolved monthly climatology. For riming and ice crystal accretion these climatologies are displayed in Fig. B.1 in the Appendix. How accurate a process needs to be represented or how drastic a simplification can be depends both on how important a process is in the model and how much the process rates vary spatially and/or temporally. Of course various other more sophisticated simplifications are possible to conceive, but since we only simplify here as a proof that simplifications are possible, we refrain from exploring these other options. The goal here is not to create a simple model (as e.g., Molteni (2003) for long simulations), but to improve interpretability of the CMPs scheme by simplifying non-influential processes. It is important to note that the simplifications and their values are not meant to be a physical estimate of what these processes do in reality. Rather, they are what we can substitute to have the model perform equally well as the detailed model. Thus, there is freedom in choosing the simplification's values, following the thought that there are superfluous degrees of freedom in these parameterizations that we replace with a single degree of freedom.

3.2.4 Historical and future simulations

To test whether the simplifications that we derive from PD simulations impede the model's ability to simulate different climate states, we perform sensitivity simulations with each of the simplifications in pre-industrial (PI) and possible future conditions. Again we keep the applied condition changes simple: for PI simulations we merely use PI aerosol emissions (ACCMIP data (Lamarque et al., 2010), from 1850, 1870, or 1900 as data was available), but everything else (greenhouse gas concentration, SST and sea ice) for the year 2003. Similarly, to represent a warmed climate state, we add a spatially resolved increase of SSTs that amounts to 4 K in the ice-free ocean mean (as in the AMIP-future4K experiments, see Webb et al. (2017)) to allow for cloud responses to warming to play out. Again the simulation setup was left unchanged apart from the prescribed SSTs and simulations were run for the year 2003.

3.3 Results

The PPE results in a response surface in the 15 parameter dimensions (12 for the P3 scheme) for each variable of interest. For the global annual mean IWP, this is illustrated in Fig. 3.6. The more order a process imposes on the response surface, the more that process influences the model output. Practically, the response surface illustrates which η_i would be most helpful to know in order to predict the variable of interest (in this case global annual mean IWP). From the first row in Fig. 3.6 a), it is clear that ice crystal autoconversion has the largest influence on IWP in the 2M scheme, as it imposes most order on the response surface. This is in line with Proske et al. (2022a). The emulated response surface in Fig. 3.6 c) reproduces this trend well. The quantitative sensitivity analysis (see Sec. 3.3.1) gives a similar result. It also indicates that ice crystal accretion is the second most important process for the global annual mean IWP, which is difficult to see in the response surface.

3.3.1 Sensitivity analysis with the 2-moment CMPs scheme (2M)

This visual analysis is helpful to illustrate the idea but the sensitivity analysis allows to quantify the sensitivities and to summarize the results more concisely for all variables (see Fig. 3.7a)). Indeed ice crystal autoconversion is the most important process for IWP (as seen in Fig. 3.6), and it also has a large influence on other variables such as ice crystal number concentration (ICNC) and hence the longwave cloud radiative effect, CC and precipitation. Other processes that the model is sensitive to include deposition and evaporation, which mostly influence CC; cloud droplet autoconversion, which reduces the LWP and hence the shortwave cloud radiative effect; and cloud droplet activation which increases cloud droplet number and mass concentration. LWP and CDNC are influenced by perturbations in cloud droplet activation, autoconversion and accretion as well as the WBF process. All of these processes are new in this analysis (compared to Proske et al. (2022a)) and strongly tied to the liquid phase. In the previous analysis riming was the only process with a direct influence on the liquid phase. This explains why riming had

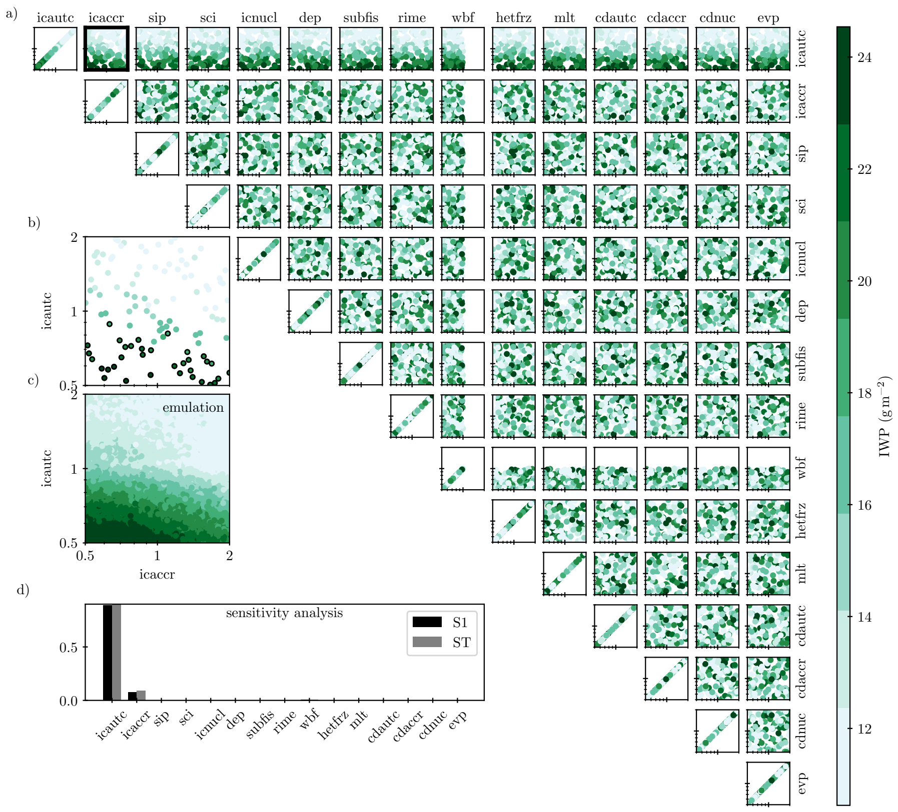

Figure 3.6: Visualisation of the model response surface for the global annual mean ice water path to perturbations in the 15 cloud microphysics processes investigated in this study. The squares show all perturbed parameter ensemble members collapsed on two process dimensions to illustrate how the model output varies with each η_i. The large inlets (**(b)** and **(c)**) highlight the two most important process dimensions, where **(c)** shows sample points drawn from the emulated surface. Additionally, in panel **(b)** the thick black edge around some circles highlights that these circles are within the range of tuning targets (Neubauer et al., 2019). The lower panel **(d)** shows the result of the quantitative sensitivity analysis. Note that $\eta_{\mathrm{wbf}} \in [0.5, 1]$ as detailed in Sec. 3.2.1.

significant effects on the global annual mean LWP and CDNC in the analysis by Proske et al. (2022a), which included only four processes in total, but is dwarfed by other processes here. This discrepancy highlights that the result of the sensitivity analysis depends on how many and which processes are included. In general, more processes mean that any process's effect may be dwarfed by another one. Similarly to ice crystal autoconversion's dominant influence on IWP, cloud droplet activation dominantly influences the global CDNC. Only ice phase processes influence the longwave cloud radiative effect, while both liquid and ice processes influence the shortwave cloud radiative effect, as expected (Lohmann and Ferrachat, 2010; Hourdin et al., 2017; Neubauer et al., 2019). Cloud cover is influenced by ice crystal and cloud droplet autoconversion, most likely via lifetime effects, as both of these processes form precipitation. Similarly, the growth of hydrometeors via deposition, which enhances precipitation, explains why that process has a negative effect on CC. The strongest influence on precipitation is by far from ice crystal autoconversion. While ice processes are known to have a large effect on precipitation (Mülmenstädt et al., 2015), the dominant role of one single process is interesting here (see discussion below).

To aid the analysis, we have added sensitivities that we expect from physical understanding of the processes into the picture. These can be understood with the aid of Fig. 3.2. For example, cloud droplet accretion converts cloud droplets and rain drops into rain drops and thereby reduces CDNC and LWP, forming precipitation and thereby reducing the lifetime of liquid clouds and hence the shortwave cloud radiative effect. For most variables and processes the physical understanding matches the result of the sensitivity analysis in sign: as expected, CDNC increases with more cloud droplet activation, and autoconversion decreases the number and mass concentration of the respective hydrometeor species. However, there are cases where physically we would expect to see a sensitivity but do not in the model results and vice versa.

On the one hand, cases where the model includes an effect that is not evident from physical understanding (circles without a colored edge in Fig. 3.7) can indicate indirect effects that are difficult to foresee. Mostly this concerns CC, the computation of which is detached from the CMPs in ECHAM-HAM, because CC formation depends on the relative humidity only (Sundqvist et al., 1989). Effects on CC from the CMPs can thus be only indirect. These take place via lifetime effects, where processes that remove crystals or droplets from the cloud and form precipitation dissolve the cloud, decrease its lifetime and thus reduce global annual mean CC. For deposition, one could have expected a direct effect on CC as deposition reduces relative humidity, but this calculation is limited to within cloud where it does not matter for the calculation of newly formed CC. However, as deposition increases ice crystal size and thus precipitation formation, it has a cloud lifetime effect and via that influences longwave cloud radiative effect (LCRE). The only process that influences CC directly via the relative humidity is evaporation of precipitating cloud droplets, which moistens the cloud free air and therefore leads to a subsequent increase in CC.

On the other hand, unexpected effects can highlight the discrepancy from physical understanding of direct effects and the adjustments that take place in the model. For example, looking at Fig. 3.2 one would expect the WBF process to increase ice and decrease CDNC and LWP, but to leave the ICNC unchanged. However, in the global annual mean we only observe an influence on ICNC, which is decreased when increasing the WBF process. Thinking in adjustments, this counterintuitive result makes sense: in the WBF process mass is transferred to the ice crystals, which therefore form sedimenting precipitation faster, hence the ICNC is reduced. The signal in IWP is likely masked out by ice crystal autoconversion, as discussed below.

Where physical understanding suggests an effect but none is found, we suspect that the influence of this particular process is masked out by another process that dominates the variable in question. In this context it is interesting to note that the physical understanding suggests either redundancies in process effects and/or counteracting processes. For example, secondary ice production, self-collection of ice and ice crystal nucleation should directly influence the same variables, where in fact secondary ice production is the reversed process of self-collection of ice. Since multiple processes are in principle able to affect the same variables, it is clear that some do this more than others, even though the magnitude of this effect is surprising. In particular, ice crystal autoconversion is the dominating influence on IWP, ICNC and the longwave cloud radiative effect. In fact, it dominates the IWP so heavily

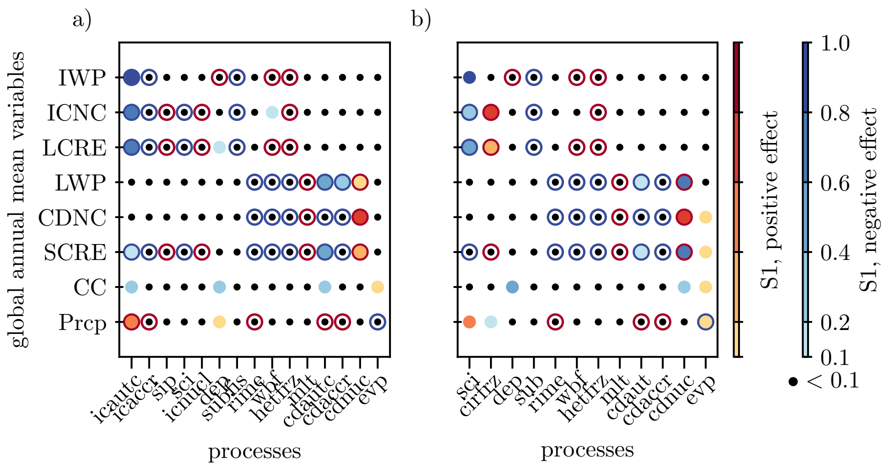

Figure 3.7: Summary of the sensitivity analysis with the **(a)** 2M and **(b)** P3 cloud microphysics schemes in ECHAM6-HAM. The sensitivity of the global annual mean variables (vertical axis; ice and liquid water path (IWP/LWP), ice crystal and cloud droplet number concentration (ICNC/CDNC), long/shortwave cloud radiative effect (LCRE/SCRE), cloud cover (CC) and total precipitation (Prcp)) to 15 (12 for the P3 scheme) investigated processes (horizontal axis, see Table 3.1) is displayed in terms of the first direct effect (S_1). Outer circles denote sensitivities we expect from physical understanding and inner circles denote the results of the global sensitivity analysis. Black dots denote $S_1 < 0.1$. Red colors indicate a positive correlation (e.g. an increase in η_{icautc} leads to an increase in precipitation), and blue colors indicate a negative correlation (e.g., an increase in η_{icautc} leads to a decrease in IWP). These correlations were estimated from the difference between the mean for $\eta_i > 1$ and $\eta_i < 1$. Note that we define the SCRE in absolute amount, meaning that more reflection of shortwave radiation translates to a stronger SCRE. The process labels are explained in Table 3.1. The corresponding sensitivity analysis of the total effects (S_T) is displayed in Fig. B.2 in Appendix B.

that in comparison no other process has a significant influence. This is discomforting since the divide between ice and precipitating snow crystals in the 2-moment scheme is somewhat artificial and solely based on size. The contribution of cloud droplet autoconversion seems to be more balanced with the other processes. This is also a result of tuning, because in the 2-moment scheme in ECHAM-HAM ice crystal autoconversion is massively increased to match tuning targets (see Table A1 in Proske et al. (2022a)), mostly that of longwave cloud radiative effect. The large sensitivity of CMPs to autoconversion has been documented before (Gettelman, 2015; White et al., 2017; Proske et al., 2022a), and accordingly it has been suggested to remove the artificial threshold conversion between ice and snow (Morrison and Milbrandt, 2015; White et al., 2017). This is the motivation behind repeating the same PPE and sensitivity analysis using the P3 scheme, which removes the strict divide between ice and snow crystals, allowing both to sediment, and thus has no need for the process of autoconversion.

3.3.2 Sensitivity analysis with the P3 CMPs scheme

To eliminate the large influence of ice crystal autoconversion, we repeat the same experiments and analysis with the P3 scheme that overcomes this somewhat artificial

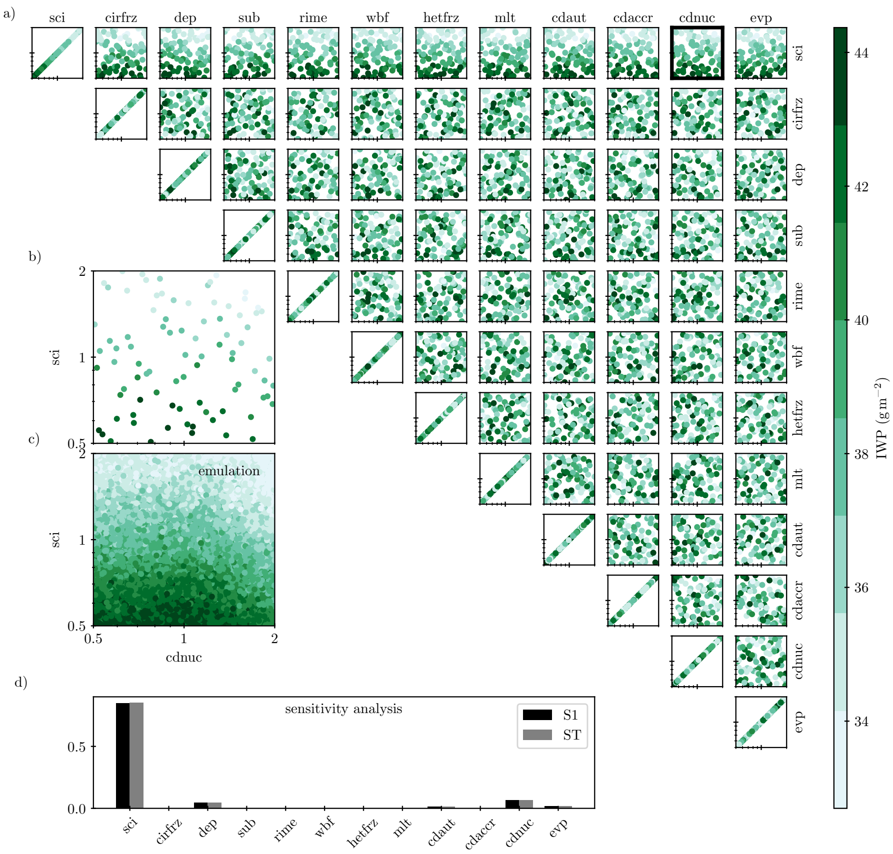

Figure 3.8: Same as Fig. 3.6, but for the P3 scheme. Acronyms for the processes are explained in Table 3.1.

process and the divide between ice crystals and snow flakes. Indeed, Fig. 3.8 shows that the influence on IWP is slightly more distributed between processes in the P3 scheme. Without ice crystal autoconversion, self-collection of ice takes over the dominating influence on IWP (with minor contributions from cloud droplet nucleation and deposition), but the longwave cloud radiative effect is dominated by nucleation in the cirrus regime. While the P3 scheme adds some sensitivities and removes others, some of the added sensitivities again oppose physical understanding. Interestingly, the influence of cloud droplet activation on LWP and thus shortwave cloud radiative effect has changed sign in the P3 analysis. A decrease in LWP makes sense in an aerosol limited regime, where increasing cloud droplet activation acts the same as increasing aerosols/cloud condensation nuclei, leading to more but still sufficiently large cloud droplets to initiate growth by the collision-coalescence process leading to precipitation and thus decreasing LWP overall.

3.3.3 Simplifications in the 2M CMPs scheme

In the 2M scheme, eight processes do not have a significant influence on any global mean variable. These processes, namely ice crystal accretion, secondary ice production, self-collection of ice, ice crystal nucleation, sublimation of falling ice and snow, riming, heterogeneous freezing and melting of sedimenting snow and ice, offer themselves for simplification. At least for sublimation, riming and heterogeneous freezing, the P3 scheme is also insensitive to them. The easiest and most drastic simplification is to remove a process or inhibit an effect entirely. This simplification is successful only for heterogeneous freezing and secondary ice production (tests removing other processes are not shown). Figure 3.9 shows that for all investigated annual mean variables, removing heterogeneous freezing and secondary ice production together (dark blue lines) causes deviations in the zonal means of mostly less than 10% at all latitudes. At some latitudes, however, ICNC decreases up to 25%. The fact that the other six processes are not simplifiable so drastically may indicate that their sensitivities are negligible compared to the dominating processes but not small enough to be removed entirely (which we investigate below and in Fig. 3.10) or that their sensitivities over the investigated range (η_i between 0.5 and 2) are not a good proxy for this drastic simplification. The next drastic simplification possibility is to set the direct effect of a process on the CMP variables (which was multiplied by η_i in the PPE) constant. This gives mostly satisfying results for the sublimation of sedimenting ice and snow and self collection of ice (light blue line), except for an underestimation of the IWP by roughly 10 % to 20 % and an underestimation of CC. For melting, this simplification gives small deviations. For riming, ice crystal accretion, ice crystal nucleation and melting, both of these simplification methods result in large deviations, which is why we tried a height-resolved monthly zonal mean climatology instead. The simplifications of riming in this manner introduces overestimations of the LWP as well as underestimations of the LCRE (green line, and yellow line for the riming simplification applied separately). Ice crystal accretion gave large deviations, mostly in ICNC, LCRE and CC (magenta line). Lastly, for ice crystal nucleation deviations are large, sometimes over 50% in the zonal mean.

From the results of the sensitivity analysis which indicated that the model is not sensitive to these eight processes, the deviations upon simplification are surprising. However, the PPE and sensitivity analysis compare all of the 12 investigated processes, meaning that the eight processes we identified for simplification are merely unimportant compared to the other processes but may not be unimportant overall. To zoom in on the sensitivities to these eight processes only, we sampled from the emulated PPE holding all other processes constant. The resulting sensitivity analysis is presented in Fig. 3.10. Ice crystal accretion now stands out as influencing IWP, riming as influencing LWP and ice crystal nucleation as influencing ICNC, LCRE, and shortwave cloud radiative effect (SCRE). This explains why the simplifications of these processes are difficult or unsuccessful in exactly those variables. Self-collection of ice and sublimation have less influence on directly affected variables and are thus easier to simplify. The model exhibits almost no sensitivity to heterogeneous freezing, melting and secondary ice production, even when zooming in on the processes like this, which explains why their simplification was successful even with the most drastic approach.

3.3.4 Testing the simplifications in historical and possible future scenarios

Whether one accepts the presented simplifications as viable depends on one's modeling purpose (Parker, 2009). However, no matter how accurate the simplifications are in present climate, for using them in a global climate model, we need to evaluate their performance in different climate states. We therefore conduct simulations with the simplifications active in a PI climate, signified by decreased PI aerosol emis-

Table 3.2: Comparison between the simplification simulations in terms of effect on aerosol radiative forcing (five year mean, difference between present day (PD) and pre-industrial (PI) aerosol states).

Simulation	Net top of the atmosphere radiation balance F_{net} (PD) ($W\,m^{-2}$)	Aerosol radiative forcing ($W\,m^{-2}$): F_{net} (PD) - F_{net} (PI)
Default	0.31	2.0
Remove hetfrz and sip	0.19	2.0
Constant subfis and sci	-0.95	1.9
Climatology rime	-0.20	2.1
Climatology icaccr	-0.40	1.8
Climatology mlt	0.058	2.0

sions, and in a future warmed climate, implemented with increased SST simulations (AMIP-future4K experiments, see Webb et al. (2017)). The simplification of ice crystal nucleation was omitted from these experiments as its performance in present-day conditions was already deemed insufficient in performance. Figures 3.9b and 3.9c compare the results of these simulations to the ones conducted in PD conditions (Fig. 3.9a). Without the simplifications (in the default simulations, black line), PI aerosols lower the CDNC drastically mostly in the Northern Hemisphere, and lower CC, LWP, ICNC, and subsequently LCRE as well. The simplified simulations mimic these changes from the default simulation but keep the deviations that they exhibit in PD conditions. Similarly, in the future simulations LWP and precipitation increase, ICNC decreases and sign of the changes in IWP and CC varies with latitude. Again the simplified simulations mimic these changes while keeping similar deviations from the default simulations. These results confirm that the simplifications we derived from PD simulations hold and can be used also in simulations of different climate states.

How one interprets the results of the scheme characterisation as well as the resulting simplifications depends on one's modeling vision (Shackley, 2001; Sundberg, 2009). In performance aspects, one needs to evaluate whether the deviations that the process simplifications cause are acceptable, and this depends on the model/projection purpose (Parker, 2009). If one wants to have a model that represents how processes behave in the real atmosphere, the unimportance of secondary ice production and heterogeneous freezing in the investigated model version is especially troublesome. In principle, the successful simplifications could mean that these processes are unimportant in the atmosphere. However, both are usually believed to be important processes for ICNC (Kanji et al., 2017; Villanueva et al., 2021; Korolev and Leisner, 2020; Kärcher et al., 2022; Qu et al., 2022) and thus the model behavior seems faulty. The insensitivity of ECHAM-HAM to heterogeneous freezing (formulations) has been documented before (Hoose et al., 2008a; Dietlicher, 2018; Dietlicher et al., 2019; Villanueva et al., 2021; Ickes et al., 2022) but never as clearly as in the present study. Our hypothesis for this model behavior is a strong seeder feeder mechanism (Roe, 2005; Seifert et al., 2009; Ansmann et al., 2009; Proske et al., 2021) in the model, meaning that ice crystal sedimentation is supplying ice crystals from cirrus clouds to lower levels so readily in the model that it renders heterogeneous freezing unimportant even as a threshold process. Of course despite careful review we can also not exclude bugs as the reason for the discrepancy between model results and understanding. These questions warrant further studies, where a creative and extended use of the emulated model response could be effective, for example, to investigate the effect of heterogeneous freezing and secondary ice production by scaling the response surface or reducing its dimensionality (as in Fig. 3.10). Additional tests have shown that for example, increasing the efficiency of heterogeneous freezing by a factor larger than $\eta_{\mathrm{hetfrz}} = 2$ allow it to influence global ICNC significantly (tests with $\eta_{\mathrm{hetfrz}} = 5$ not shown).

In terms of understanding the model it is interesting to note that only ice processes have potential for simplification. Tapiador et al. (2019) state that given the nonlinear chaotic nature of CMPs schemes it is "surprising that the microphysics produce consistent results" and attribute this to them being "buffered systems" (Stevens and Feingold, 2009), meaning that "if one of the processes in the MP is poorly modeled the others may take the lead and compensate." We have already mentioned the redundancies in processes' effects. It seems like these redundancies and buffering play out more in the ice processes with some processes masking out the effects of others. This implies that the warm phase CMPs are more balanced and urges us to reevaluate the balance in the ice phase CMPs in the ECHAM6-HAM GCM.

3.4 Summary, conclusions and outlook

Using an emulated PPE of process efficiency in the CMPs in ECHAM-HAM, we characterize and compare the 2M and P3 CMPs schemes and conduct sensitivity analysis. In the 2M scheme, the model is sensitive to about half of the investigated processes, with ice crystal autoconversion clearly dominating the ice phase variables. The warm phase sensitivities are more balanced. Since the P3 scheme removes the artificial divide between ice crystals and snow flakes, other processes than ice autoconversion influence the global ice variables. Where sensitivities do not match physical understanding, this is either due to other processes dominating the sensitivity or adjustments to the perturbed processes in the model. For example, in the global annual mean, the WBF process decreases ICNC, because it leads to larger ice crystals that sediment more readily. In comparison to all other processes, seven of the investigated processes offer themselves for simplification. However, the sensitivity to some of these is masked in the total analysis and only revealed when excluding more prominent processes from the emulated model response. Which deviations from simplifications one can accept for the CMPs is dependent on the intended use case of the model. In principle, insensitivity can be interpreted either as the process being not important also in reality, or hinting at something being wrong in the model. In the case of heterogeneous freezing and secondary ice production, to which the model is the least sensitive, we think the latter is the case. In any case, these results highlight the strength of our analysis: It allows us to highlight model deficiencies and to identify simplifications.

It is important to note that we investigate the model as it is used. Many factors in the model setup probably influence this analysis, for example the tuning state (see Table B.1), the model time step (Gettelman et al., 2013; Barrett et al., 2019; Zhu et al., 2021; Zarzycki, 2022), the ordering of processes (Donahue and Caldwell, 2018), the resolution, of course the CMPs scheme choice but also the other schemes in the model that interact with the CMPs (Yang et al., 2022). Thus, the sensitivity analysis results are not transferable to another model (version). However, the comparison of the 2M and P3 scheme highlights that there is some generality in the analysis, especially considering that the schemes have structural differences as well, for example, sequential versus parallel operator splitting and the subtimestepping in the P3 scheme. Also, our methodology lends itself as a tool to compare different models, model versions or schemes and could thus help to elucidate the aforementioned effects.

In this analysis we regard only global annual means. Proske et al. (2022a) have investigated a PPE of only four CMP processes and shown that there a regional or seasonal analysis gives sensitivities in line with the global analysis. As we add onto their analysis, we do not expect regional effects to contradict our conclusions and thus refrain from that analysis. An interesting addition to our work would be the investigation of physically finer grained variables, such as a distinction between mixed-phase and cirrus temperature ICNC (since total ICNC is dominated by cirrus clouds, there is e.g., the possibility of a larger influence of heterogeneous freezing on mixed-phase temperature clouds). Similarly, our analysis is based on annual mean values, but variability in these values may exhibit different sensitivities to the same processes.

We have chosen the range of our perturbations, $\eta_i \in [0.5, 2]$, the same for all processes in order to keep them comparable and investigate the effect of modifications or simplifications. If one would like to cover the range of process rates, the uncertainty of the processes or the effect of a specific simplification directly, one would need to find meaningful ranges for each of the processes individually. For example, one could argue that processes affecting the number concentrations would need to have larger ranges than the ones affecting mass, as number concentrations of ice crystals range several orders of magnitudes. This may make the ranges more meaningful and thus aid the analysis, but would include a host of insufficiently constrained assumptions. In our case the analysis is exploratory, to characterize the scheme as it is. Therefore we choose to keep the perturbations the same for each process. We only include the magnitudes of modifications in single processes afterward in testing the different simplification possibilities. Similarly, for CMP processes that act sporadically with process rates that vary by orders of magnitude, it may be more sensible to perturb how often they occur instead of perturbing their magnitude. However, as we find that the results of our simplifications are in line with our sensitivity analysis, we conclude that our perturbations were one right exploratory tool.

This study presents the method of using a PPE and sensitivity analysis to explore a model in a new light: we use the sensitivity analysis to characterize a model scheme and explore possibilities for simplification. Our analysis highlights that one needs to first understand the model and the parameterizations at hand. Only then one is able to interpret process studies or improve parameterizations. Adjustments in the model often have unexpected effects that conflict with physical understanding. For example, the role of heterogeneous ice nucleation is an active study area (see e.g., Kärcher et al. (2022) and Maloney et al. (2022)), but our study suggests that more detailed parameterizations are of no use in ECHAM-HAM until its insensitivity to heterogeneous ice nucleation is explained.

In particular, the fact that we find processes that do not change the model's behavior in PD, PI or warming conditions, highlights that we have more processes in the model than we can constrain (Morrison et al., 2020). Depending on one's modeling vision (Shackley, 2001; Sundberg, 2009) and the purpose of one's model (Parker, 2009), one may interpret this finding and what to follow from it differently. Detailed process representations may be needed for certain model purposes, but there is no point in a scheme containing a large number of involved processes without utility, which merely make the scheme complicated (Baartman et al., 2020). As Held (2005) states, it is fruitless to elaborate details "in ways that have no practical consequences or no hope of confronting data." At the very least, scheme complexity and complicatedness need to be taken into account in model selection and development (Larsen et al., 2016).

The need to understand model behavior is generating creative studies that elucidate problematic model effects (Fiddes et al., 2022). This study adds a method for this with exemplary characterisation of two CMPs schemes. The scheme characterisation is helpful for model development. One may use it backwards, prescribing ranges for output variables such as global mean CC, to generate possible process ranges, that is, η_i. Thereby it could also be used for tuning the model, where one may choose to extend the ranges of the PPE or extrapolate the emulator to widen the phase space. To generalize the gained understanding, our analysis method can be used to compare schemes and models, to investigate which model sensitivities are robust.

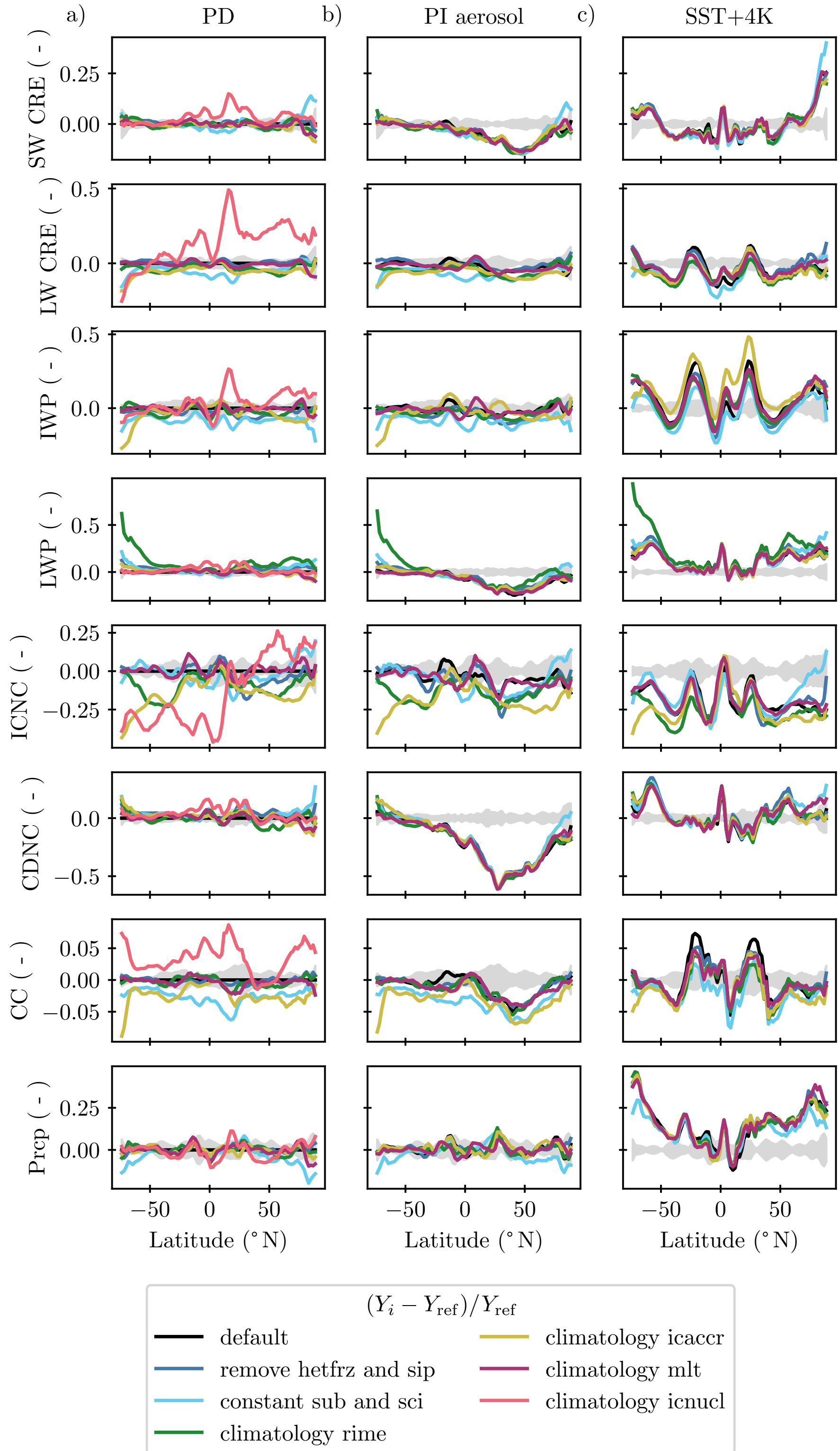

Figure 3.9: Relative deviations of the simplified model versions from the default in terms of the zonal 5 years mean (variables vertically integrated where applicable) for **(a)** present day (PD), **(b)** pre-industrial (PI) conditions (PI aerosol emissions) and **(c)** possible future conditions (realized with a 4 K increased sea surface temperatures). The gray shading indicates the inter annual variability of the PD default simulation. Process labels are explained in Table 3.1, and variables in Appendix D. Note that the southernmost latitudes are excluded in this Figure as their small absolute values cause deceptively large relative deviations.

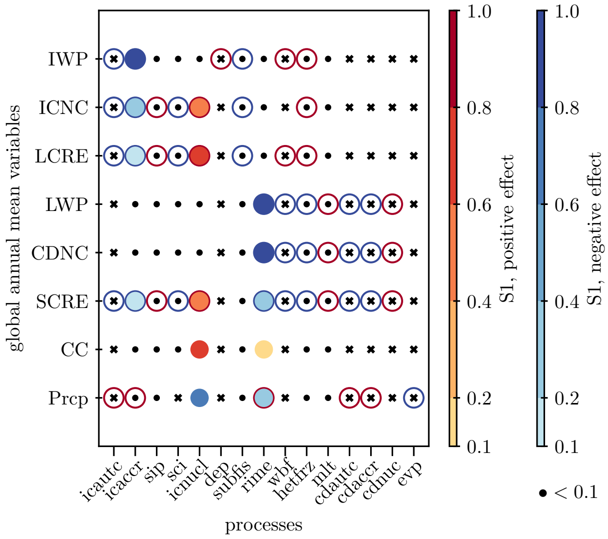

Figure 3.10: As Fig. 3.7 a, but holding all processes except the ones identified for simplification (heterogeneous freezing, secondary ice production, sublimation of sedimenting ice and snow, self collection of ice, riming, ice crystal accretion, melting and ice crystal nucleation) constant when sampling from the emulated perturbed parameter ensemble. Processes held constant are indicated by small crosses instead of dots that indicate small sensitivity.

Open Research Section The ECHAM-HAMMOZ model is freely available to the scientific community under the HAMMOZ Software License Agreement, which defines the conditions under which the model can be used. The specific version of the code used for this study is archived in the ECHAM-HAMMOZ SVN repository[2]. More information can be found on the HAMMOZ website[3]. Analysis and plotting scripts are archived at https://doi.org/10.5281/zenodo.7375978 (Proske et al., 2023c). Generated data is archived at https://doi.org/10.5281/zenodo.7376058 (Proske et al., 2023b). The PyDOE library (tisimst, 2021) was used for Latin Hypercube Sampling, ESEm (Watson-Parris et al., 2021c; Watson-Parris et al., 2021a) for the construction of the emulator, and SALib (Usher et al., 2020) for the sensitivity analysis.

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Throughout this study, the programming languages CDO (Schulzweida, 2018) and Python (Python Software Foundation, www.python.org) were used to handle data and analyze it. The visualizations have made ample use of Paul Tol's color blind friendly color schemes (Tol, 2021). The ECHAM-HAMMOZ model is developed by a consortium composed of ETH Zurich, Max Planck Institut für Meteorologie, Forschungszentrum Jülich, University of Oxford, the Finnish Meteorological Institute and the Leibniz Institute for Tropospheric Research, and managed by the Leibniz Institute for Tropospheric Research (TROPOS). ECHAM-HAM simulations were performed on the ETH Zürich Euler cluster. This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant 821205 (FORCeS).

[2]at /root/echam6-hammoz/tags/papers/2022/Proske_et_al_2022_JAMES_for-review_2M and /root/echam6-hammoz/tags/papers/2022/Proske_et_al_2022_JAMES_for-review_P3

[3]https://redmine.hammoz.ethz.ch/projects/hammoz, last access: 30 November 2022

4

Developing a climatological simplification of aerosols to enter the cloud microphysics of a global climate model

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Abstract Aerosol particles influence cloud formation and properties. Hence climate models that aim for a physical representation of the climate system include aerosol modules. In order to represent more and more processes and aerosol species, their representation has grown increasingly detailed. However, depending on one's modeling purpose, the increased model complexity may not be beneficial, for example because it hinders understanding of model behaviour. Hence we develop a simplification in the form of a climatology of aerosol concentrations. In one approach, the climatology prescribes properties important for cloud droplet and ice crystal formation, the gateways for aerosols to enter the model cloud microphysics scheme. Another approach prescribes aerosol mass and number concentrations in general. Both climatologies are derived from full ECHAM-HAM simulations and can serve to replace the HAM aerosol module and thus drastically simplify the aerosol treatment. The first simplification reduces computational model time by roughly 65%. However, the naive mean climatological treatment needs improvement to give

results that are satisfyingly close to the full model. We find that mean CCN concentrations yield an underestimation of CDNC in the Southern Ocean, which we can reduce by allowing only CCN at cloud base (which have experienced hygroscopic growth in these conditions) to enter the climatology. This highlights the value of the simplification approach in pointing to unexpected model behaviour and providing a new perspective for its study and model development.

4.1 Introduction

Climate models are used both to understand the Earth system and to project its changing behaviour. In building models, their representativeness and realism are taken to be important indicators of model quality. In this view, the models' scope has historically expanded (Edwards, 2011) to include various Earth system compartments and components, from land surface properties to atmospheric chemistry. Aerosol particles are one such Earth system component that has started to be represented in climate models since the late 1990s (CarbonBrief, 2018). Aerosol particles are liquid or solid particles suspended in air, ranging from black carbon to sea salt or bacteria. They are important for the climate system, both with direct effects, such as by absorbing or scattering radiation, and indirect effects via their interaction with clouds (Lohmann and Feichter, 2005; Storelvmo, 2017).

In particular, aerosols serve as cloud condensation nuclei (CCN) and ice nucleating particles (INPs) and thereby facilitate water phase changes in the atmosphere. Small droplets have a high curvature, which increases their saturation vapor pressure (Kelvin effect). Such high supersaturations are not reached in the atmosphere. Hence, cloud droplets do not nucleate homogeneously. Instead, cloud droplets nucleate on CCN. A hygroscopic aerosol particle takes up water when exposed to humid air (hygroscopic growth). As it grows, the CCN dissolves in the forming solution droplet and thereby acts as a solvent to lower the droplets' saturation vapour pressure (Raoult effect). Köhler theory combines the Kelvin and Raoult effect, which results in an equilibrium saturation pressure curve with a maximum at the so-called activation radius (see Fig. 4.2). Once a CCN reaches this supersaturation and grows beyond the activation radius, it will continue to grow even with decreased supersaturation, and is hence termed an activated cloud droplet.

Similarly, the energy barrier associated with freezing is too high for cloud droplets to freeze homogeneously in the atmosphere. Until −35 °C cloud droplets freeze only heterogeneously on an INP, which serves to lower the energy barrier associated with the freezing process (Murray et al., 2012; Lohmann et al., 2016; Kanji et al., 2017). At lower temperatures, cloud droplets freeze homogeneously, without the aid of an INP. The salts dissolved in smaller solution droplets lead to a freezing point depression. Thus, solution droplets freeze homogeneously only at low temperatures or high supersaturations with respect to ice. Alternatively, they can freeze heterogeneously with the aid of an INP (Lohmann et al., 2016).

Thus aerosols influence cloud properties. For example, when aerosol particle concentrations are higher, more cloud droplets form. Given the same amount of liquid water in a cloud, they have a smaller size. This delays precipitation formation, increasing cloud lifetime (Albrecht effect, Albrecht (1989) and Storelvmo (2017)). However, clouds also influence aerosol particle concentrations, e.g. with precipitation removing aerosol from the atmosphere via wet scavenging. These aerosol-cloud interactions are numerous, challenging to quantify and thus their resulting forcing is associated with a large uncertainty (Boucher et al., 2013; Bellouin et al., 2020; Bender, 2020). This is because the scales involved range from the interaction of micrometer particles to effects on the global energy balance. Observations to quantify these interactions at a global scale are inherently difficult (Quaas et al., 2020). For climate modeling, the small scales involved require that the aerosol and cloud microphysical processes are parameterized. These parameterizations are inherently associated with underconstrained degrees of freedom and uncertainty. For example, an intercomparison conducted by Fanourgakis et al. (2019) shows that there is substantial disagreement in the CCN concentrations simulated by different global models.

The climate modeling community has responded to the challenges of aerosol and cloud microphysics (CMPs) research by expanding their models to account for an increasing variety of processes and compounds. This approach is grounded in the reductionist idea that a complex system can be decomposed into its parts, which then all need to be represented. While this serves a representative vision of modeling, the increasing model complexity can arguably be counterproductive for the heuristic modeling vision, which employs models to generate understanding (see Sec. 1.3.3).

Thus the representative complexity paradigm in environmental modeling has come under challenge. For example, Cox et al. (2006) developed a systematic approach to identify excess process complexity. By automatically replacing variables with constants in the code, they generated many simplified model variants. Comparing their results, they identified redundancies or overparameterizations. This approach has been successfully performed for example on wheat and soil models (Cox et al., 2006; Crout et al., 2009; 2014). Working with the ECHAM-HAM CMPs module, Proske et al. (2022a) have introduced an approach that varies process efficiencies to test the models' sensitivity to these processes and thereby identify potential for simplification. Proske et al. (2023a) applied this method to 15 out of 17 processes in the CMPs module and were able to simplify 7 of them.

For aerosol modules, various process sensitivity studies have been reported, but without a direct tie to model simplifications (see e.g. Schutgens and Stier (2014) for an extensive aerosol pathway analysis). Instead, aerosol module simplifications tend to be more drastic. For example, Liu et al. (2012) and Ghan et al. (2012) reduced the number of modes in their aerosol module MAM (part of CAM5) from 7 to 3 modes while still achieving satisfying performance in model results. Similarly, Zhu et al. (2022) developed a parameterization of dry effective aerosol radius based on the mass of two species. This allowed them to use only a one moment (mass) prognostic representation and deduce the zeroth moment (number) at negligible computational expense. Furthermore, Ghan et al. (2013) developed a one dimensional model with physical aerosol and cloud processes included to aid in the exploration of how parameter uncertainty travels through to ACI uncertainty. Stevens et al. (2017) developed a plume climatology of anthropogenic aerosol based on the model- and observation derived MACv2 climatology. Their climatological representation MACv2-SP was analytically based and consisted of only 9 plumes, but gave good agreements to the full MACv2 climatology. They highlight its use case in comparing aerosol responses in different models. Also, Fiedler et al. (2019a) applied this fast MACv2-SP climatology in a scenario investigation. Presently, Weiss et al. (2023) are developing a simplified version of the HAM module, called HAMlite, by reducing aerosol tracers and imposing fixed aerosol composition. Number concentrations are still computed prognostically, but the predefined species composition allows to pre-compute radiative properties. This allows the scheme to be used in convection-resolving model simulations.

The process of model simplification may seem counter-intuitive at first: we are used to taking model expanse and complexity as a sign for model quality. Yet any simplification sacrifices the representative depth of a model. However, the representativeness of a given model is but one goal of model development. Other goals include predictive capability and the generation of understanding (see Sec. 1.3.3). The modeling visions of Sec. 1.3.3 may indicate conflicting avenues for model development goals. On the one hand, model complexity is encompassed by the representative vision. On the other hand, it makes models and their results more difficult to interpret and thus it harms the heuristic vision of model use for generating understanding. This conflict is what we aim to address with our simplification work.

One might object that simplifications may appear harmful even for the model's ability to supply understanding. For example, if one is interested in the process of aerosol particle coagulation, a model using a CCN climatology would not seem to be of much use. However, the simplification of one model part allows for easier investigation of other model parts, in our example e.g. cloud droplet coagulation. Also, a simplification of the process under study may help understanding, e.g. in identifying which factors influence a process and by enabling clearer sensitivity studies. When unsatisfying simplification results guide the scientific exploration, the model itself is pointing the developer towards the important processes or behaviour that shape the model response. Thus, attempts at drastic simplifications may open up new perspectives on the model understanding and development problem.

We develop a climatology of a) CCN that serves as the connection between the aerosol particles and the CMPs and b) aerosol mass and number concentrations. Both climatologies in combination with a pre-existing climatology of aerosol radiative effects can replace the aerosol module HAM. Such a top-down approach, of investigating how the model reacts to changes in aerosols, may be more effective than a tedious bottom-up approach of elaborating all possible processes, as Stevens et al. (2017) argue as well. Using the climatology allows to isolate remaining processes and their effects and study associated uncertainties. The climatology we develop and test is based on full-HAM model output. We demonstrate that this approach works in principle and discuss which features are required in the climatology. This gauges the possibilities for the use of an observation-based climatology in the future, which would satisfy both the representative and the heuristic vision while avoiding representative complexity. Most importantly, as we demonstrate, the development of the climatology already opens up new avenues for understanding.

Our approach departs from the representative approach that has dominated Earth system model development and fueled an ever increasing model complexity. To be clear, our simplifications do not attempt to judge any process as unimportant in reality. Rather, the model is our object of study. Where our findings deviate from physical understanding, this difference needs to be investigated and offers an avenue for model development. While our simplifications sacrifice representativeness for interpretability, the development for more comprehensive models may continue alongside, creating a model family of various complexity, where one may choose a configuration based on a given study's purpose. At the same time, our approach also

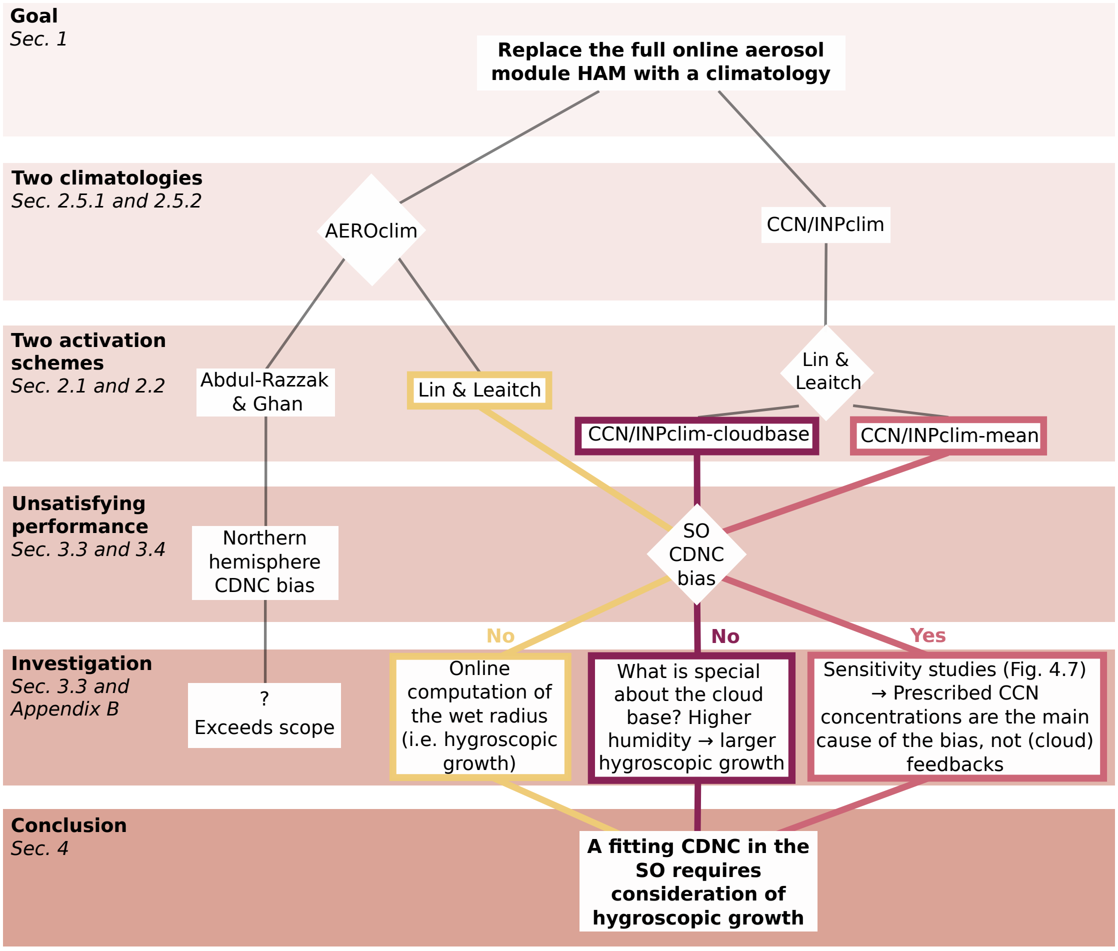


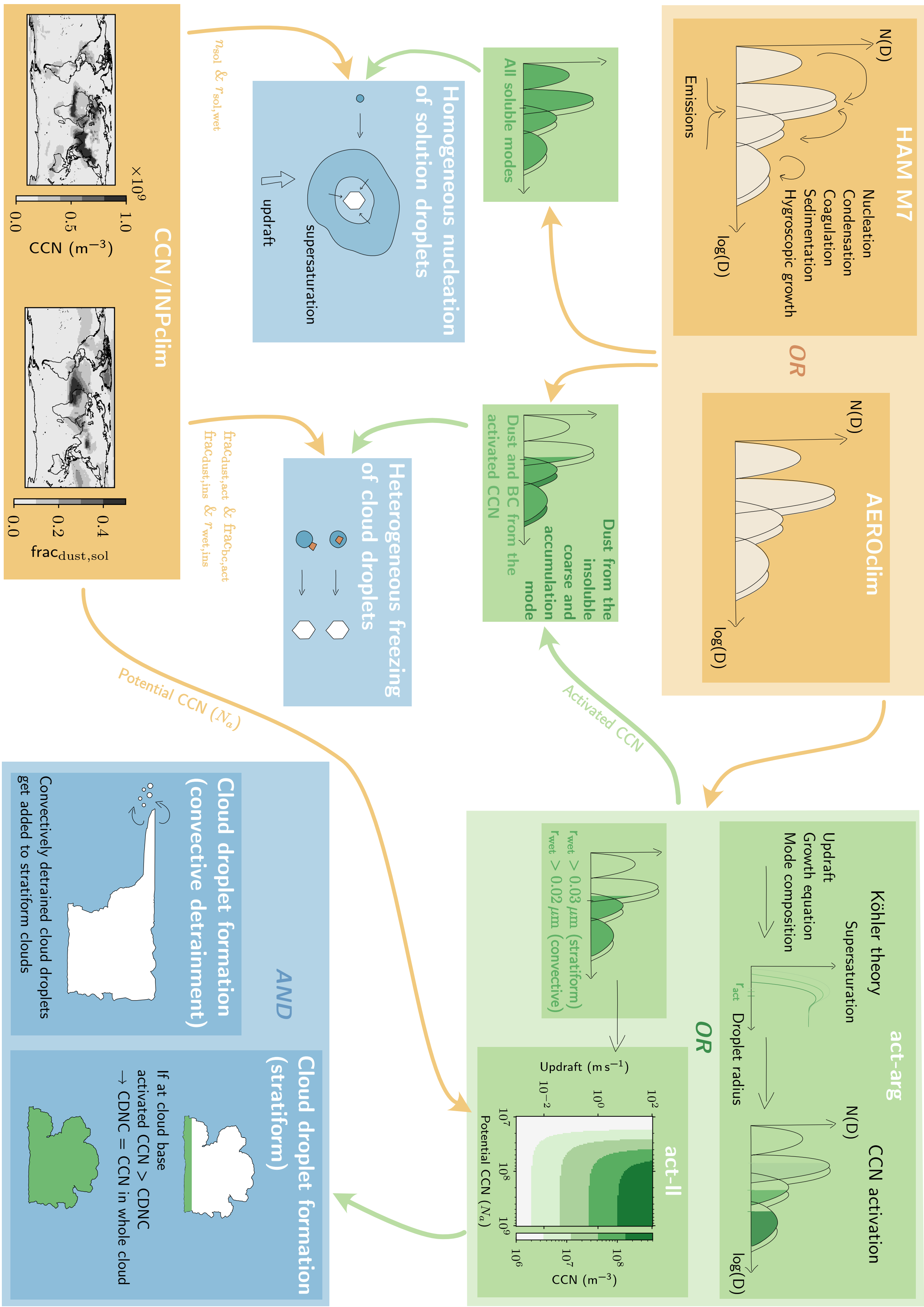
Figure 4.1: Flowchart illustrating our investigation of the different climatology versions.

satisfies the predictive vision of model development. In our simplification attempts we strive for equifinality (Beven, 2006; Beven and Freer, 2001), meaning that the simplified model produces results similar enough to the full model for the purpose at hand, thereby providing equal predictive quality. Because the CCN climatology allows to replace the whole aerosol module HAM, it incurs large reductions in the model's run time. This may be used to save costs, run more or longer simulations, detail other processes, or increase the model's resolution.

The approach and results of this study are outlined in Fig. 4.1. The following section describes the aerosol climate model ECHAM-HAM, the process implementations relevant to this study and the two CCN/aerosol climatology implementations (Sec. 4.2). In the presentation and discussion of results in Sec. 4.3, we describe the effects of both climatologies. We also detail the investigative process that co-evolved with the development of the climatology, highlighting how the approach of simplification generates model understanding. Section 4.4 discusses this approach and points out possible use cases of the CCN climatology.

4.2 Methods

This study employs the aerosol-climate model ECHAM6.3-HAM2.3 (Neubauer et al. (2019) and Tegen et al. (2019), ECHAM-HAM hereafter), in the same configuration



(Caption on next page.)

Figure 4.2: Illustration of the points where aerosols influence cloud microphysics in the model and where hence the AEROclim and CCN/INPclim approaches are applied. Both climatologies are derived from a full HAM default simulation, which diagnoses monthly mean tracer diagnostics or potential CCN (and the other variables indicated in the illustration), respectively. Note that CCN/INPclim can be used only with the Lin & Leaitch (*act-ll*) and not with the Abdul-Razzak & Ghan activation scheme (*act-arg*). $\mathrm{frac_{dust/bc,act}}$ is the fraction of dust/black carbon in activated aerosol, $\mathrm{frac_{dust,ins}}$ is the fraction of dust in the insoluble coarse and accumulation mode, $\mathrm{r_{dust,wet}}$ is the wet radius of dust, $\mathrm{n_{sol}}$ is the number concentration of soluble aerosol and $\mathrm{r_{sol,wet}}$ is its wet radius. The CCN and INP climatology plots are illustrative, for one month and level (the climatologies really are four dimensional, resolved in space and time (in the form of monthly means)).

as in Proske et al. (2022a). Its aerosol module HAM was implemented by Stier et al. (2005) (updated to HAM2 by Zhang et al. (2012)) using the 7 mode aerosol module M7 from Vignati et al. (2004). Aerosols of varying composition are grouped into 7 lognormal size distribution modes, which are distinguished by size and solubility (see Fig. 4.2). Various process treatments are included in HAM, for example condensation or coagulation moving particles between modes. Hygroscopic growth of aerosol particles is implemented using Köhler theory with a prescribed hygroscopicity parameter for each substance, following Petters and Kreidenweis (2007) (Zhang et al., 2012). The 2-moment CMPs scheme prognostically computes ice crystal and cloud droplet mass and number and diagnoses rain and snow mass concentrations (Lohmann et al., 2007). For a detailed description of the included cloud microphysical processes see Chapter 3. As in the real atmosphere, in ECHAM-HAM the aerosols influence CMPs by serving as CCN or INPs in cloud droplet activation and ice crystal nucleation. There are two cloud droplet activation parameterizations implemented into ECHAM-HAM (see Table C.1 for their separate tunings).

Lin & Leaitch cloud droplet activation

The cloud droplet activation following Lin and Leaitch (1997) (**act-ll** in the following) was implemented into ECHAM-HAM by Lohmann et al. (2007) (see Fig. 1.2). It empirically relates the number of nucleated cloud droplets, $\mathrm{CDNC_{act}}$, to the aerosol number concentration and updraft:

$$\mathrm{CDNC_{act}} = 0.1 \times 10^{10} \cdot \left(\frac{N_\mathrm{a} \cdot w}{w + 2.3 \times 10^{-10}\,\mathrm{m^4/s} \cdot N_\mathrm{a}} \right)^{1.27} \tag{4.1}$$

Here, for N_a ECHAM uses the number concentration of aerosols particles with wet radii $> 0.03\,\mu\mathrm{m}$[1]. Thus N_a first needs to be derived from the soluble aerosol size distributions in HAM (see Fig. 4.2). The updraft w is calculated from the mean updraft, the turbulent kinetic energy and contributions from the convective available potential energy (see Lohmann et al. (2007) for details).

Equation 4.1 is an empirical relationship derived in Lin and Leaitch (1997). They used aerosol and cloud droplet measurements from a field study in the North

[1]Note that this is different from the $0.035\,\mu\mathrm{m}$ cut-off radius that is stated in Lohmann et al. (2007), which Lohmann et al. (2008) changed to $0.03\,\mu\mathrm{m}$ to accomodate tuning constraints. This cutoff refers to stratiform clouds. For detrained convective clouds, the cutoff is radii $> 0.02\,\mu\mathrm{m}$ (introduced as $0.025\,\mu\mathrm{m}$ in Lohmann (2008)).

Atlantic[2] to evaluate two cloud droplet activation parameterizations, of Ghan (Ghan et al., 1993; Ghan et al., 1995) and Abdul-Razzak (Abdul-Razzak et al., 1998). Both parameterizations were found to underestimate measured CDNC, but if one used the maximal updraft as input, both were able to predict the maximum measured CDNC well. Thus Lin and Leaitch (1997) proposed to use these parameterizations to calculate the maximum CDNC and gave an empirical relationship to compute the mean CDNC. In their ECHAM-HAM implementation, Lohmann et al. (2007) used this empirical relationship in combination with the Ghan parameterization because the Abdul-Razzak formulation relied on supersaturations which may be unrealistic at the model grid scale (personal communication Ulrike Lohmann).

Abdul-Razzak & Ghan cloud droplet activation

The Abdul-Razzak & Ghan cloud droplet activation parameterization (**act-arg** in the following, introduced in Stier (2016) and Lohmann and Neubauer (2018) (see Tegen et al. (2019))) is explicitly based on Köhler theory. In HAM, each of the seven modes has a different composition. Thus, Köhler coefficients need to be computed for each soluble mode separately (using Abdul-Razzak et al. (1998, Eq. 5) and Abdul-Razzak and Ghan (2000, Eq. 3 and 4); the nucleation mode is excluded from activation). From these coefficients and the updraft velocity, a maximum supersaturation is calculated. This is translated to an activation radius for each mode via the mode radius and its corresponding critical supersaturation (Abdul-Razzak and Ghan, 2000, Eq. 12). Subsequently, all aerosols larger than the critical radius are activated into potential activated cloud droplets ($\mathrm{CDNC_{act}}$) for each mode.

Activated cloud droplets enter the cloud microphysics

Whether the potentially activated cloud droplets calculated in one of the previous parameterizations actually produce new cloud droplets is determined in the CMPs module. For all cloud bases at liquid or mixed-phase cloud conditions, it evaluates whether $\mathrm{CDNC_{act}}$ exceeds the present CDNC. If this is the case, the CDNC at cloud base and throughout all cloud levels above is set to $\mathrm{CDNC_{act}}$ that was calculated for the cloud base. This approach resembles the adiabatic ascent of an air parcel with cloud droplet activation occuring mainly at cloud base.

Ice crystal nucleation in ECHAM-HAM

In ECHAM-HAM, ice nucleation mechanisms are parameterized as follows:

- **Heterogeneous freezing at mixed-phase temperatures** ($0\,^\circ\mathrm{C} > T > -35\,^\circ\mathrm{C}$) was introduced in Lohmann and Diehl (2006) and distinguishes two types of heterogeneous freezing, which are considered to be important in the atmosphere: Dust from the coarse and accumulation insoluble modes aids in

[2] The field study was the North Atlantic Regional Experiment in 1993. Lin and Leaitch (1997) used data from 14 flights in and around stratus clouds over the Bay of Fundy and the Gulf of Maine in August and September. This illustrates the mismatch in complexity between the 28 tracer HAM module and the 15 processes in the CMPs module that are connected through a parameterization that is based on data sampled in a constrained timeframe and location. The $2.3 \times 10^{-10}\,\mathrm{m^4/s}$ factor is empirically based and was transmitted via personal communication from Richard Leaitch to Ulrike Lohmann.

contact nucleation (Lohmann and Diehl (2006) and Hoose et al. (2008a), following Young (1974), Cotton et al. (1986), and Levkov et al. (1995b)). Its number concentration is multiplied with an efficiency factor that accounts for the species specific temperature dependent INP efficiency. For this factor, the dust is assumed to be composed of montmorillonite (values given in Hoose et al. (2008a, Table 1)). Both mineral dust and hydrophilic black carbon participate in **immersion freezing** (Lohmann and Diehl (2006) and Hoose et al. (2008a) following Diehl and Wurzler (2004)). For their number concentration, the soluble accumulation and coarse mode of both species are used (Lohmann and Neubauer, 2018). In practice, the fraction derived from dividing their activated concentration by the activated CCN number concentration, is used in the parameterization. Again, this is multiplied by an efficiency to mirror the temperature dependent INP ability of the individual species. Again, for the mineral dust, montmorillonite composition is assumed.

- **Homogeneous freezing of cloud droplets at cirrus temperatures** ($T < -35\,^{\circ}\mathrm{C}$) is realised simply by converting all clouds droplets to ice crystals at these temperatures.
- **Homogeneous freezing of solution droplets at cirrus temperatures** ($T < -35\,^{\circ}\mathrm{C}$) was introduced in Kärcher and Lohmann (2002b) and Lohmann and Kärcher (2002). It uses the soluble aerosol number concentration and radius from HAM as input. Since homogeneous ice nucleation may take place at high supersaturations with respect to ice, it solves for the competition between updraft creating supersaturation and crystal growth depleting it. Heterogeneous freezing of solution droplets at cirrus temperatures ($T < -35\,^{\circ}\mathrm{C}$) has been implemented into ECHAM-HAM previously (Lohmann et al., 2008), but is not used in this study.

4.2.1 The aerosol/CCN climatology

CCN/INP climatology (CCN/INPclim)

To create the aerosol cloud climatology that enters *act-ll*, the number of potential CCN is diagnosed from a full HAM simulation. In this way, only one CCN concentration instead of all HAM tracers needs to be saved, while the activation that takes into account updraft can still take place (see Fig. 4.2). This total number is thus independent of the aerosol composition. Apart from the CCN concentration, the soluble aerosol particle concentrations (without a cutoff radius) as well as their mode radii are supplied to the homogeneous freezing of solution droplets. The particle concentration is determined from the potentially available CCN that is also used as input to *act-ll*. This introduces a deviation from the default setup, where the entire Aitken, accumulation and coarse soluble modes are used, without any lower limit for their radii. In processing the output from the default setup, the maximum of the monthly mean CCN over all conditions and those at cloud base was used to create the monthly mean, 3D resolved climatology (CCN/INPclim-cloudbase), i.e.

$$\mathrm{MAX}(\mathrm{MEAN}(\mathrm{CCN}_{\mathrm{all}}), \mathrm{MEAN}(\mathrm{CCN}_{\mathrm{at\,cloudbase}})).$$

This is because the cloud base condition (which for cloud droplet activation is restricted to $T > -35\,^{\circ}\mathrm{C}$) leads to an underestimation of CCN at cirrus temperatures and thus for the homogeneous freezing of solution droplets. Hence our climatology uses the maximum of the mean CCN concentration over all conditions and the mean cloud base CCN concentration.

Since the CMPs scheme uses CCN only at cloud base for activation, CCN/INP-clim-cloudbase represents cloud droplet activation conditions in the model more specifically. The cloud base condition is the relevant one because in the current implementation activation is limited to cloud base and the enhanced CDNC is taken to be the same at higher cloud levels (see Fig. 4.2). Using only the mean CCN concentration (CCN_{all}) was also tested (CCN/INPclim-mean). In fact, investigating the difference between CCN/INPclim-mean and -cloudbase allowed us to formulate the more appropriate conditions for a CCN climatology (see Sec. 4.3.3).

The treatment of heterogeneous contact freezing of CDs requires the fraction of insoluble dust aerosol as well as its radius as input. They are also diagnosed from the full HAM simulation. For immersion freezing, the fraction of dust and black carbon aerosol of the activated aerosol is used. These quantities are used as 3D monthly mean fields in the climatology.

Aerosol climatology (AEROclim)

Act-arg requires detailed composition as well as number concentrations for each mode. Hence, to be able to use the parameterization in its present form, all these properties needed to be prescribed and using the CCN/INPclim approach does not work for *act-arg*. In the implementation, we opted for a pragmatic approach: in the default simulation, all aerosol tracers (mass and number for each mode and species) were diagnosed as monthly means. In the climatology simulations these were prescribed and all processes that would change the tracers' concentrations were deactivated. AEROclim can of course also be used for *act-ll*.

Note that AEROclim supplies monthly mean aerosol concentrations, which are used to compute aerosol properties online. In the case of non-linear computations, the quantities computed from monthly means will not be equal to the monthly mean of those quantities. Thus one can expect deviations between CCN/INPclim (which uses mean quantities) and AEROclim (which computes these quantities from the mean).

Aerosol radiation climatology

Aerosol particles' effects on climate are not limited to clouds, but they also exhibit a radiative effect on their own. Thus, when we replace HAM with CCN/INPclim, the radiative aerosol effect requires a special treatment as well. Different versions of a climatological treatment of aerosol radiative properties have been implemented into ECHAM-HAM already. For AEROclim, radiative properties can be computed online from the supplied aerosol concentrations. For CCN/INPclim, we use the Max Planck Institute Aerosol Climatology (MAC-v1) developed by Kinne et al. (2013), which is based on both photometer observations and model data (ARclim). Alternatively, for sensitivity tests we also use a setup with no aerosol radiative effect (NoAR).

4.2.2 Historical and future simulations

To test whether the simplifications that we derive from present-day (PD) simulations (run for 2003 or 2003-2012) impede the model's ability to simulate different climate states, we perform sensitivity simulations with each of the simplifications in pre-industrial (PI) and possible future conditions. Again we keep the applied condition changes simple: for PI simulations we merely use PI aerosol emissions (ACCMIP data (Lamarque et al., 2010), from 1850, 1870, or 1900 as data was available), but everything else (greenhouse gas concentration, SST and sea ice) for the year 2003. Similarly, to represent a warmed climate state, we add a spatially resolved increase of SSTs that amounts to 4 K in the ice-free ocean mean (as in the AMIP-future4K experiments, see Webb et al. (2017)) to allow for cloud responses to warming. Again the simulation setup was left unchanged apart from the prescribed SSTs and simulations were run for the year 2003.

4.3 Results and discussion

Applying CCN/INPclim to replace HAM yields surprisingly equifinal results to a full ECHAM-HAMMOZ simulation. Figure 4.4 shows that the climatology causes some positive deviations in cloud droplet number concentration (CDNC) between −30 °N and 30 °N in the liquid cloud regime, as well as at around 50 °N in the mixed-phase cloud regime. At −50 °N, CDNC is underestimated by CCN/INPclim-cloudbase in both temperature regimes. While these deviations are larger than the inter-annual variation of the default simulation, they are small in relative terms, remaining roughly $< 25\%$. The deviations in CDNC translate to deviations in the liquid water path (LWP), which are even smaller in relative terms. In the ice phase, CCN/INPclim-cloudbase causes significant yet small positive deviations in the mixed-phase ice crystal number concentration (ICNC), restricted to the northern hemisphere. In the cirrus regime, CCN/INPclim-cloudbase leads to increases in ICNC at roughly 10 °N and 10 °S of the equator. These changes in ICNC result from a combination of the CCN/INPclim-cloudbase modifications in aerosols supplied to CCN activation, INPs and homogeneous freezing of solution droplets (see Sec. 4.3.2). The ice number changes do not translate to significant ice mass changes (see ice water path, IWP), except for the positive deviation at roughly 10 °S. This in turn causes a positive deviation in longwave cloud radiative effect (LCRE).

Whether the deviations between the full aerosol scheme and the climatology are judged to be acceptable depends on one's modeling purpose. CCN/INPclim offers large savings in computational time. Figure 4.3 illustrates that HAM takes up more than 40 % of the computational time (excluding writing output). In comparison, the 2-moment CMPs scheme takes up roughly 10 % and the transformations between the spectral and cartesian grid take up about 5 %. In AEROclim aerosol concentrations are prescribed and excluded from advection, but still HAM needs to compute aerosol properties from the concentrations. Thus the simulation takes longer than CCN/INPclim. However, there is room for additional time savings: some properties like the wet radius are updated multiple times in the HAM routines, which may be reduced since processes affecting the wet radius are deactivated in AEROclim. In addition, some properties may be pre-computed with the frequency of the climatological input, similar to how Weiss et al. (2023) treat aerosol radiative processes. The single

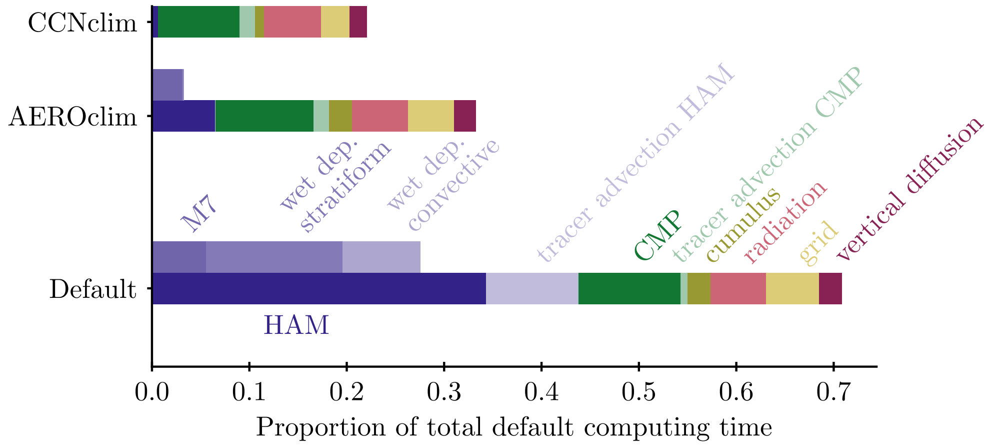


Figure 4.3: Relative computing time associated with the most expensive model parts, compared between a default and a CCN/INPclim model run (15 days, without writing output). The M7 aerosol microphysics are highlighted as part of the HAM aerosol module. Wet deposition is the most expensive single process and is called both in the stratiform and the convective cloud microphysics. Tracer advection handles both 28 aerosol and 2 cloud microphysics tracers and is divided here accordingly. In the case of CCN/INPclim and AEROclim the CMP tracer advection is not shared with HAM and thus the overhead is attributed solely to the CMP tracer advection timing, making it appear larger. *grid* names the transformations between the spectral and cartesian grid coordinates. For AEROclim, some HAM property computations are still executed, based on prescribed aerosol concentrations.

most expensive process related to aerosol treatment is the wet deposition, which is called twice, in the stratiform and the convective CMPs scheme. Thus, switching the wet deposition scheme from the more complex scheme of Croft et al. (2010) (size-dependent in-cloud and below-cloud scavenging) to a simpler scheme would enable large time savings of up to 20 %. Running the model with CCN/INPclim instead of HAM reduces the simulation time by 65 % (not shown, simulations for 15 months and including the writing of output with our standard requirements).

For predictive purposes, the large savings in computational expenses may outweigh the deviations in cloud particle concentrations. In fact, these may be minimized with further development of the climatology and tuning of the model, which we have not attempted. For our purpose of understanding model behaviour, CCN/INPclim-cloudbase results are deemed sufficiently similar to the default simulation to allow for a comparison. In particular, its development towards achieving such similarity opened up new perspectives (see Sec. 4.3.3).

4.3.1 Effect of the radiation climatology

Replacing HAM requires not only a new treatment of cloud active aerosols, but also replacing their radiative effects. In ECHAM, one can choose between interactive HAM aerosols (default), or climatologically prescribed aerosol radiative effects (ARclim, used in CCN/INPclim-cloudbase case), or no aerosol radiative effect (ARclim0). To be able to judge the effect of the radiative climatology separately, Figure 4.4 compares the full HAM simulation with two that use HAM while treating only radiation climatologically. In terms of cloud variables, the ARclim and ARclim0 results re-

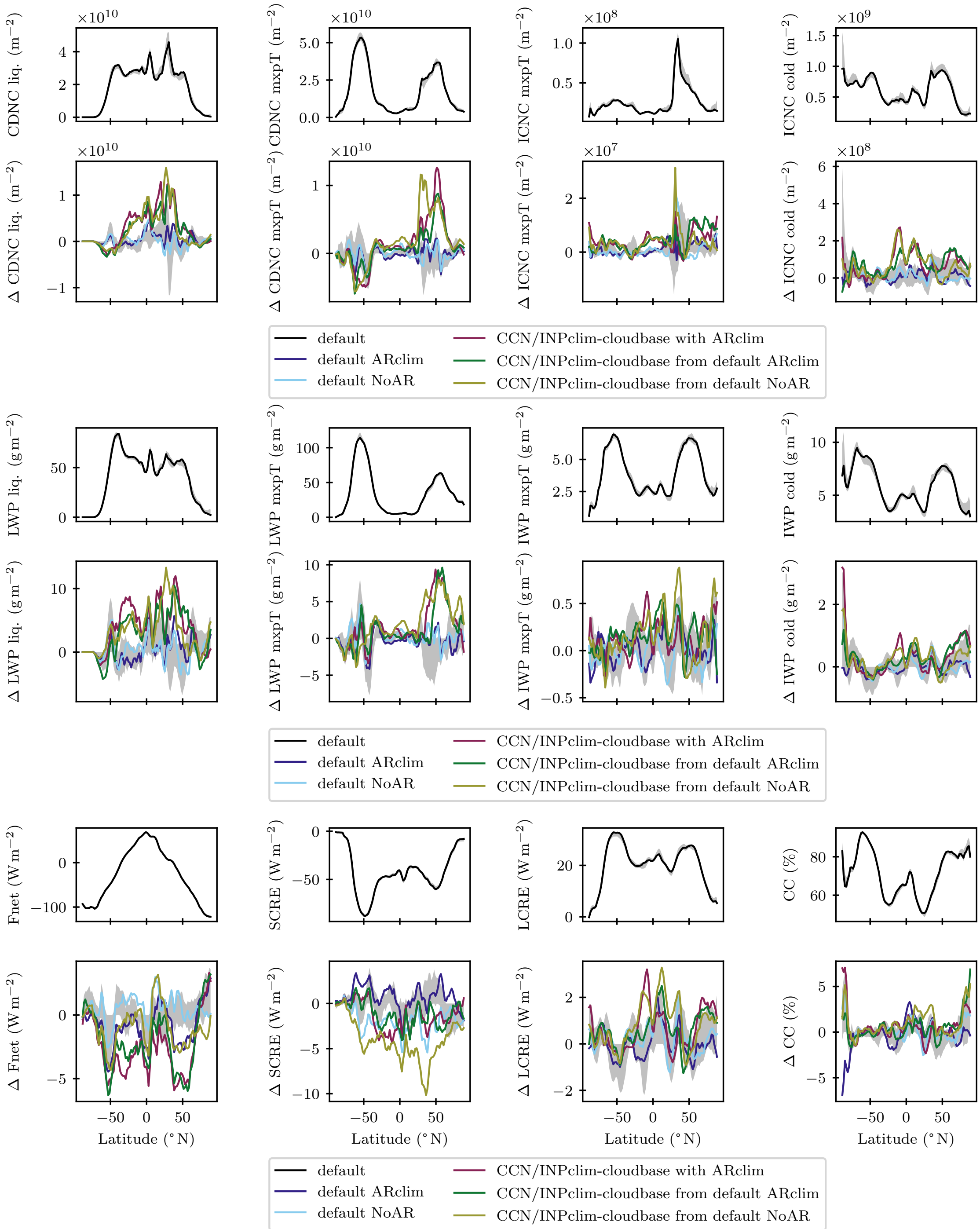


Figure 4.4: Zonal annual means, highlighting the effect of using a climatology for radiation. Uneven rows show absolute values for default simulations, and even rows show the deviations to the default simulation. All simulations are for the year 2003, and the grey shading indicates the maximum deviation from the 2003 default simulation in annual means between 2003 and 2012. The CCN/INPclim-cloudbase was either derived from a full HAM simulation (CCN/INPclim-cloudbase ARclim3) or from default simulations that in turn used an aerosol radiative climatology (CCN/INPclim-cloudbase from default ARclim or NoAR), where then the same radiative aerosol treatment was employed for the CCN/INPclim simulation.

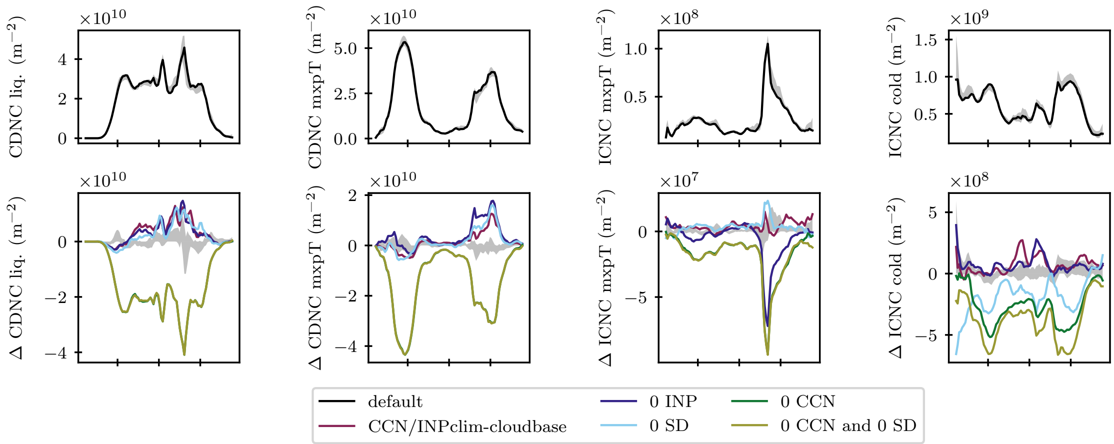
main within or close to inter-annual variability. Only for ICNC at mixed-phase temperatures, there is a large positive deviation at around 30 °N. The northern mid-latitudes are influenced by high concentrations of Saharan dust aerosol, which is radiatively active. The temperature changes induced by a change in the aerosol radiative climatology may influence heterogeneous freezing, because that is temperature dependent. Also, note that the ICNC at mixed-phase temperature is orders of magnitude smaller than the other hydrometeor concentrations, which are less affected by ARclim (in Fig. 4.4 for cold ICNC and both CDNCs the dark blue line remains within inter-annual variability). We thus do not expect the radiative treatment of aerosols to impact the performance of the aerosol cloud climatology. This is mostly the case: CCN/INPclim-cloudbase simulations with the climatologies derived from the three different radiative treatment simulations give only slightly different results for cloud properties. The most pronounced difference arises from using the CCN/INPclim-cloudbase climatology without radiative treatment of aerosols (light green in Fig. 4.4), which exhibits an increase in CDNC and LWP at around 30 °N and in turn increases the magnitude of the shortwave cloud radiative effect (SCRE). Also, in this simulation ICNC at cirrus temperatures is decreased at latitudes around 30 °N compared to the other CCN/INPclim-cloudbase simulations. Similarly as for heterogeneous freezing, the missing radiative effect of dust aerosols may induce local temperature perturbations and thus turbulent kinetic energy changes, to which the homogeneous freezing of solution droplets is particularly sensitive (Kuebbeler et al., 2012). In the CCN/INPclim-cloudbase configuration, the model may be deprived of some regulating feedbacks to these temperature changes, leading to larger differences between the radiatively different variants of CCN/INPclim than in the default variants.

To sum up, the radiative aerosol climatology does not yield much difference in zonal mean cloud variables compared to the full HAM, but the combination of CCN/INPclim-cloudbase with ARclim enhances the differences. Thus, getting a perfect climatology for both CMPs and radiation requires developing both together. However, the climatological treatment of aerosol radiative effects does not affect the main observations in the CCN/INPclim-cloudbase case. This eases our interpretation of CCN/INPclim-cloudbase and allows for a fair evaluation of CCN/INPclim-cloudbase against the default.

4.3.2 Separate effects of the CCN/INP climatology

To test and illustrate the effect of CCN/INPclim-cloudbase on the various ways in which aerosol particles seed cloud particles, we conducted simulations in which each of the INP, CCN and solution droplet effects was set to 0 separately (for details on the processes see Fig. 4.2).

Disabling heterogeneous freezing by setting INP concentrations to zero (*0 INP* in Fig. 4.5) decreases mixed-phase ICNC and increases CDNC in mid-latitudes. This is particularly pronounced at 30 °N, where high concentrations of ice-nucleating Saharan dust particles are prevalent. The confined and overall small effect of heterogeneous freezing of cloud droplets on the hydrological cycle agrees with what previous studies have found for ECHAM (Hoose et al. (2008a), Dietlicher (2018), Dietlicher et al. (2019), Villanueva et al. (2021), Ickes et al. (2022), Ickes et al. (2023a), and Chadzelek (2023), see also Chapter 3). The division by temperature regimes



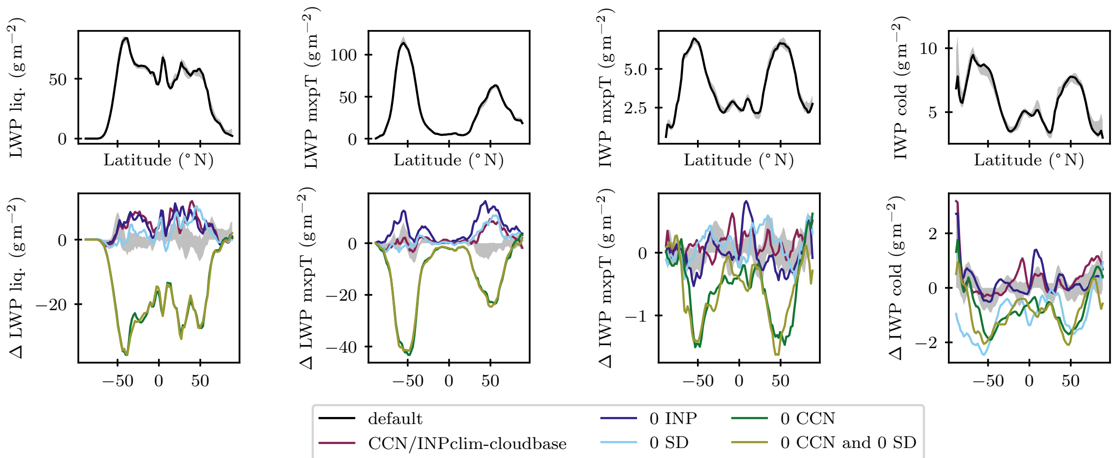


Figure 4.5: As Fig. 4.4, but for the CCN/INPclim-cloudbase sensitivity simulations where parts of the climatology were set to 0.

highlights that this effect is hidden in the global mean ICNC, since this quantity is dominated by cirrus ICNC (hence the insensitivity to heterogeneous freezing in Chapter 3).

Aerosol particle concentrations in the model are also used to derive solution droplet concentrations, where solution droplets freeze homogeneously in the cirrus regime. Accordingly, when we set these to zero in the climatology (*0 SD* in Fig. 4.5), cirrus ICNC decrease dramatically. Other cloud particle concentrations are unaffected by this change.

On the contrary, supplying zero aerosol particle concentration for cloud droplet activation (*0 CCN* in Fig. 4.5) dramatically affects all mass and number particle concentrations, decreasing both water and ice. This test illustrates the functioning of our CCN/INPclim-cloudbase climatology. However, one may wonder why significant water and ice mass mixing ratios are retained even without any CCN. This highlights the role of the CDNC minimum value in ECHAM, which serves to enforce a minimal number concentration in order to avoid unrealistically large cloud droplets. Note that the total water (sum of water vapour, liquid and ice water mixing ratios) is conserved and that condensation is calculated from a saturation adjustment approach, i.e. cloud liquid water is also formed in the absence of CCN. In clouds with liquid water content, that minimum CDNC is dynamically calculated in our setup (see Sec. 2.2). Thus, the liquid water mass is distributed over a small number of cloud droplets instead of being reduced to zero.

4.3.3 CCN/INPclim development

The difference between the two approaches to generate CCN/INPclim (CCN/INPclim-mean and CCN/INPclim-cloudbase) illustrates how the development of simplifications may force us to question and update our model understanding (illustrated in Fig. 4.1). Figure 4.6 shows that the results of the two approaches deviate most for Southern Ocean (SO) CDNC. This is strongly underestimated when employing CCN/INPclim-mean. Representing liquid clouds in the SO is a particularly common challenge for climate models in general (Bodas-Salcedo et al., 2016; Kay et al., 2016; McCluskey et al., 2023), but it is not obvious why the mean climatology would deviate so strongly from the default simulation.

Investigating this difference further, Figure C.3 shows that indeed this deviation is restricted to the SO (by this term we mean latitudes between $-40\,^{\circ}$N and $-80\,^{\circ}$N in the following). The underlying potential CCN concentrations show an overestimation of CCN by CCN/INPclim-cloudbase in the SO, compared to the default. While both CCN and CDNC have strong seasonal differences in the SO, the relative differences with CCN/INPclim-mean or -cloudbase do not. These results indicate that CDNC in the SO can only be achieved with a monthly CCN climatology that overestimates CCN concentrations relative to the mean, regardless of season or baseline concentration. It is clear that the activation of CCN into cloud droplets is a process where large concentrations are important, because these have the potential to raise CDNC (because activated CCN can only raise CDNC if their concentration is higher than the pre-existing CDNC). However, it is not a priori clear why the CCN difference is especially large in the SO, leading to large differences in CDNC there. To understand this behaviour, we have conducted various sensitivity simulations that help to exclude some hypotheses (see Appendix C.2 and Fig. C.1). These sensitivity

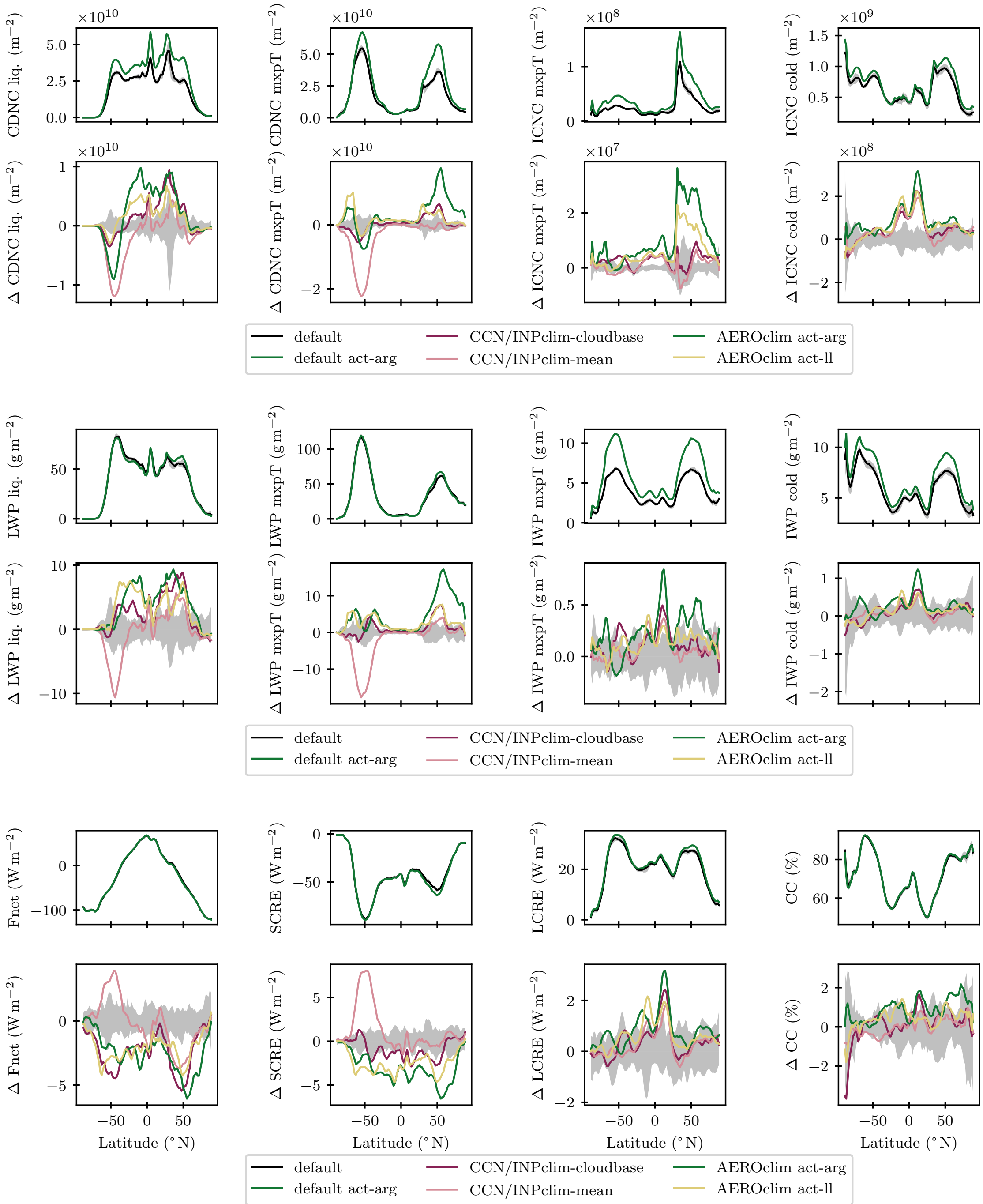


Figure 4.6: Zonal annual means, highlighting the effect of the different climatology variants. Uneven rows show absolute values for default simulations, and even rows show the deviations to the default simulation. *AEROclim act-arg* is shown in terms of difference to the *default act-arg* simulation. All values are annual means for the years 2003-2012, and the grey shading indicates the maximum deviation from the 2003 default simulation in annual means between 2003 and 2012. The climatologies were derived from the 10 year default simulations.

simulations helped us to exclude interactions with the CMPs or other feedbacks and influences as the source of the SO bias. They clearly point to the prescribed CCN themselves being the reason for the CDNC discrepancy. In parallel, we had developed AEROclim, which prescribed aerosol rather than CCN concentrations (see Sec. 4.3.4). Using AEROclim with *act-ll* alleviated a SO discrepancy similarly to CCN/INPclim-cloudbase. This reinforced the idea that the bias in the SO does not stem from the use of a monthly climatology per se, but that the prescribed CCN values must be at fault.

The key to the SO bias proved to be the question: "why do cloud base conditions lead to higher CCN concentrations"? In clouds, the humidity is larger than outside of clouds. For soluble aerosol particles, increased humidity implies hygroscopic growth. Whether aerosols have experienced hygroscopic growth is relevant for *act-ll*, because it relies on the wet aerosol radius to estimate the concentration of CCN (see Fig. 4.2). Indeed, Fig. C.2 shows that diagnosing CCN over all conditions implies a smaller wet radius than diagnosing it only at cloud bases. Hence, diagnosed CCN concentrations are smaller. This effect is especially pronounced in the SO. This can be explained by the larger relative humidity over oceans in general, as well as by the aerosol species composition. As stated above, the SO aerosol is dominated by sulfate and sea salt, which are much more hygroscopic than other aerosol species such as mineral dust (Lohmann et al., 2016). In the AEROclim case, the change in wet radii due to hygroscopic growth and the size cut-off are performed in online calculations. Thus, online computed CCN concentrations take cloud base conditions into account. In sum, in order to use a CCN climatology for *act-ll*, hygroscopic growth of particles needs to be taken into account (as in AEROclim), or CCN need to be diagnosed at cloud base conditions already (as in CCN/INPclim-cloudbase).

4.3.4 AEROclim

AEROclim alleviates the SO bias, but instead, zonal mean CDNC and LWP values are rather overestimated with AEROclim. For *act-arg*, AEROclim overestimates CDNC by about a third in the Northern Hemisphere, between 25 °N and 75 °N. This bias may be subjected to similar tests as the ones we have performed for the SO bias above to elucidate its underlying cause. In particular, one would need to investigate the error that is introduced with AEROclim, where aerosol quantities such as the radius are computed from monthly mean concentrations using nonlinear relations.

4.3.5 CCN climatologies in different climate states

Figure 4.7 illustrates the performance of the climatologically simplified model with respect to the full HAM default. The different climate states manifest themselves e.g. in a decrease in northern hemisphere CDNC and LWP for the pre-industrial simulation. Regardless of these differences in the default simulations, the change induced by the simplification is similar for these different climate states. The overestimation of CDNC and LWP in the northern hemisphere decreases in pre-industrial climate. We attribute this to the decrease in absolute numbers that is present in the default simulation, Also, the role of minimum CDNC is bound to be more prominent in PI conditions and the minimum condition is present in both the full HAM and simplified model version. In the predictive vision, simulations in varying climate states serve

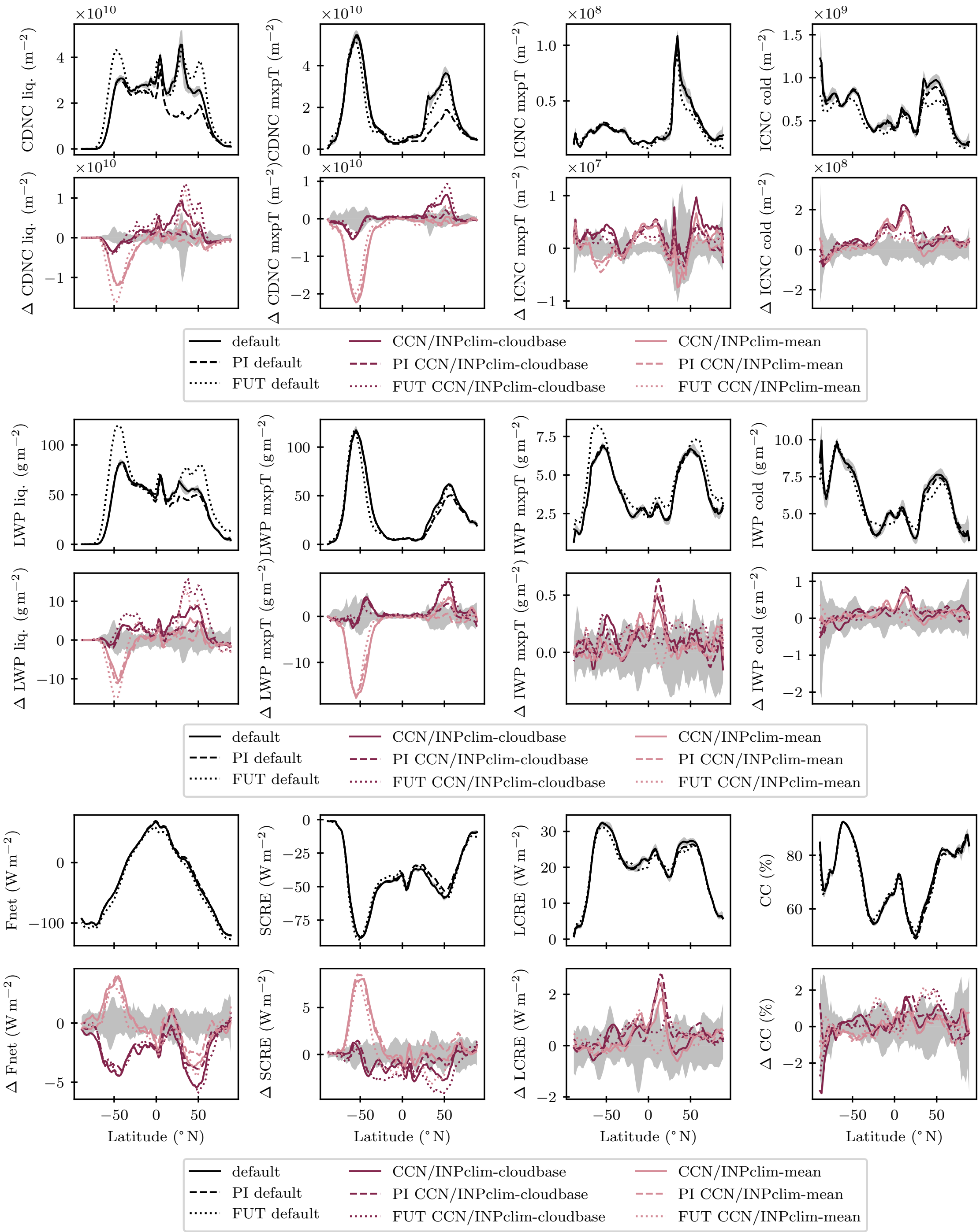


Figure 4.7: As Fig. 4.6, but comparing the different variants of the aerosol/CCN climatology for different climatological states. There are three default simulations (present-day, pre-industrial and plus 4 K conditions, as described in Sec. 4.2.2) in the uneven rows. The differences in the even rows are with respect to the respective climatological default state. See Fig. C.4 for the AEROclim simulations, and Fig. C.5 for a direct comparison of the differences between climate states.

Table 4.1: Comparison between the simplification simulations in terms of effect on aerosol radiative forcing (ARF) and climate sensitivity, computed from 10-year means. ARF is the difference between present day (PD) and pre-industrial (PI) radiation balances (F_{net} (PD) - F_{net} (PI)). The climate sensitivity $\lambda = \frac{\Delta T_{sfc}}{-(F_{net,FUT} - F_{net,PD})}$ is computed from the change in surface temperature ΔT_{sfc}. All other quantities (first four columns) are given for the PD simulation. F_{net} is the net top of the atmosphere radiation balance. Cloud droplet number concentration (CDNC) and liquid water path (LWP) are vertically integrated. The simulations were conducted as detailed in Sec. 4.2.2, with the default simulations from the respective climate state providing the climatological input to the sensitivity simulations (the 10-year mean of CCN/INclim or AEROclim was used). Fig. 4.7 and C.4 and C.5 in Appendix C.3 show the simulation results in more detail.

Simulation	F_{net} ($W\,m^{-2}$)	CDNC ($W\,m^{-2}$)	LWP ($W\,m^{-2}$)	SCRE ($W\,m^{-2}$)	ARF ($W\,m^{-2}$)	λ ($K\,m^2\,W^{-1}$)
default act-ll	0.57	2.5	82	-49	-1.7	0.47
CCN/INclim-mean	0.25	2.1	80	-48	-1.9	0.44
CCN/INclim-cloudbase	-2.0	2.6	86	-50	-2.3	0.47
AEROclim act-ll	-1.7	2.7	88	-52	-2.0	0.45
default act-arg	0.18	3.3	82	-50	-1.9	0.46
AEROclim act-arg	-2.5	3.7	91	-54	-1.9	0.46

to infer the reaction of the climate system to such changes. Table 4.1 summarizes the aerosol radiative forcing (ARF) and climate sensitivity (λ) as two key quantities of interest in this regard (see e.g. Bellouin et al. (2020)). λ is well preserved by the simplifications. ARF exhibits differences of up to $\approx 35\%$, which are still small compared for example to the probability distribution of ARF presented in Bellouin et al. (2020). This is despite a strong mismatch between default and simplified model in the radiation balance at the top of the atmosphere in all climate states (see Fig. 4.7). Since the CCN climatologies are a drastic simplification, some mismatch is to be expected. As Table 4.1 shows, this mismatch is only to some part due to changes in CDNC, LWP and subsequently SCRE. Comparing to Fig. 4.4, it becomes clear that the climatology of the aerosol radiative effect adds to the discrepancy in radiative balance as well. However, the fact that the mismatch between full HAM and CCN/INPclim is consistent between climate states suggests that on the one hand, it could likely be alleviated by tuning the CCN/INPclim model or improving the radiation climatology. On the other hand, differences between climate states are not affected by the mismatch, and thus the ability of the model to serve in studies of climate change (sensitivity) is preserved in principle. Of course, if one's objective is to study the changes induced by changing aerosol concentrations in detail, a detailed aerosol model will probably suit that purpose better.

4.4 Summary, conclusions and outlook

We have simplified the aerosol module HAM by using it to generate a climatology. The climatology then serves as input to the interfaces from aerosols to CMPs. We have developed two versions of the climatology, one that prescribes CCN and INPs and can only be used for the empirical Lin & Leaitch cloud droplet activation scheme, and one that prescribes aerosol mass and number concentrations that can also be used with the Köhler theory based Abdul-Razzak & Ghan scheme. For both versions we could develop a climatology that globally gives promising results for our purpose of studying clouds. Regarding the simplifications fitness' for simulations in a different climate, Fig. 4.7, C.4 and C.5 in Appendix C.3 show that the use of the climatologies inflicts no structural error in different climate states. The differences induced by the simplifications in relation to the default are mostly within inter-annual variability of each other in different climates. At the same time, differences between default simulations for different climates are large, confirming that they can serve as test cases. Table 4.1 shows that the simplifications preserve estimates of climate sensitivity, but exhibit differences in aerosol radiative forcing of up to $\approx 35\%$ (for CCN/INPclim). The fact that we do not achieve equifinality in present day conditions and aerosol forcing highlights that the full complexity of the aerosol scheme has merit in the sense that it is not fully replaceable in a naively simple way. However, the climatologies and the tuning of the results to the default model can certainly be improved (see the present day radiative forcing in Table 4.1). We did not tune the simplification variants on purpose, to facilitate a clear comparison. Thus, this work demonstrates that such drastic simplifications of aerosol treatment are possible.

The simplifications result in large computing time savings of roughly 65%. This suggests the use of the climatologies in settings where computational time is limited as e.g. for long climate simulations, high resolution simulations or large ensembles. We have also claimed that simplifications can enhance the interpretability of a given model. An explicit aerosol treatment may be necessary for example for studies of their health impacts and air pollution. In our case, our interest lies in studying the modeled clouds and their properties. Thus, for this purpose it is a strength of our simplifications that they allow us to isolate and investigate only the cloud response to aerosols and not the feedback response of aerosols.

In addition, we have gained knowledge on which features of such a climatology are important. In terms of CDNC, results similar to the default could only be obtained with climatologies that take into account hygroscopic growth at cloud base conditions, which implies higher CCN concentrations. The CCN/INPclim gives satisfying results only when using CCN concentrations at cloud base to generate it. The mean CCN over all conditions at all times is smaller and results in a large underestimation of CDNC in the SO. With sensitivity experiments we have excluded various cloud feedbacks and related factors as reasons for this behaviour. This lead us to conclude that in the SO CCN vary with cloud base conditions. We can explain this with hygroscopic growth, which increases the wet radius of aerosols in more humid cloud conditions and hence leads to higher CCN concentrations at cloud base with the *act-ll* scheme. This finding has important implications for the general simplification of using a CCN climatology. Either, one would need to take hygroscopic growth on top of the prescribed CCN (as AEROclim) into account, or use a climatology that is derived from cloudy conditions already (as CCN/INPclim-cloudbase). The difficulty we had in interpreting the CCN/INPclim-mean model behaviour points to another strength of the simplifications. While developing simplifications the models forces us to look at parts that are important to the model itself. Instead of being guided by our a priori believes (which in our case pointed towards time variability or precipitation feedbacks), simplifications thus allow for a change of perspective that may provide fresh insights.

More aerosol climatologies for use in climate models have been developed previously. It is important to stress that our climatologies are not meant to be generally applicable. Rather, we propose the process of simplification as a way to gain a new perspective on model behaviour and the simplified model as an explorative tool for further study. This distinguishes our climatologies from the MACv2SP climatology developed by Stevens et al. (2017). Their climatology is analytical, which enhances its flexibility, the clearness of its assumptions and the possibilities for porting it to different models. Our climatology is meant for use in ECHAM with the goal of making its model results equifinal to the default ECHAM-HAM configuration. As such, not the single realisation of our climatology is important, but we have rather developed the model code to easily derive and employ new climatologies. This allows the kind of sensitivity studies we used to investigate the SO behaviour, which can be helpful in adapting to new model versions and investigating their differences. Further, MACv2SP is restricted to anthropogenic aerosols and prescribes a change to CDNC directly. We take into account all of HAM's (soluble) aerosols. We specifically prescribe either aerosol or potential CCN that enter the cloud droplet activation schemes online and thus keep e.g. the updraft dependence.

4.4.1 Outlook

Our climatologies are explorative and meant to aid understanding. However, the results are encouraging to the idea that for the purpose of studying clouds, the full aerosol module HAM is replaceable with a climatology. This opens the door to use observationally developed climatologies in the same setup. In this way, representative complexity could be replaced with a representative climatology. In fact, an observation-based CCN climatology may be more representative than the full HAM model itself, as the latter is known to exclude e.g. aerosol species such as nitrate, whose effect would be present in observations. Such observation-based CCN climatologies already exist. For example, Choudhury and Tesche (2022) derived one from the lidar on the satellite CALIPSO. Importantly, our study shows that the use of mean CCN climatologies will not suffice. An additional treatment of hygroscopic growth is needed, especially in the SO. To this end, one approach to be tested is to apply the difference between CCN/INclim-cloudbase and CCN/INclim-mean to scale and adapt an observation-based climatology for use in ECHAM-HAM.

Alternatively, one may modify CCN/INclim-cloudbase to tune it towards observations, to test ECHAM-HAM sensitivities towards this more representative CCN climatology. Note that observation-based climatologies limit research to present day aerosol conditions. In addition, using them for *act-arg* would require more detailed information than potential CCN concentrations on the side of the climatologies. Other model-derived CCN climatologies (as e.g. from Costa-Surós et al. (2020)) could address these concerns and may be used where their origin is thought to be superior to ECHAM-HAM-derived ones in epistemic terms. Also, by using these climatologies as input for the *act-ll* configuration, one could further elucidate the sensitivity of ECHAM towards CCN. Similarly, the simplified model version may be compared to the single moment CMPs scheme that is available for ECHAM, where CDNC is prescribed, to spotlight the role of activation in the model.

Of course our developed climatologies can be improved upon or made more sophisticated. For example, allowing for wet scavenging with a relaxation back to the climatology as it was implemented by Costa-Surós et al. (2020) in their ICON Large Eddy Simulations, would enable a reaction of CCN concentrations to cloud behaviour. However, the climatology is engineered to provide adequate results in CDNC, and not to give a best estimate of CCN concentrations (CCN/INPclim-mean would for example be more apt for at least providing the model's best estimate). Hence, in its present form, also a direct comparison of CCN/INPclim-cloudbase to observational CCN concentrations, for example to judge the model performance, would go against its purpose. Just as MACv2SP, our parameterization is meant to be a reference climatology for the effect of CCN on clouds, and "not a reference aerosol climatology" (Stevens et al., 2017).

Instead, the simplified modules allow for an easier comparison between models by eliminating differences in details. For example, cloud microphysical schemes may be compared more easily between two models using the same CCN climatology. Our implementation of the climatologies also enables easily devised sensitivity studies, for example using a different time resolution for the climatologies. In particular, AEROclim opens up many possibilities for sensitivity experiments, for example by setting single prescribed variables to 0. Thus our approach also has potential for model development. It highlights what variables or features are important for model performance, and can serve to detect unintended behaviour or mistakes in the code. Importantly, it shows the benefit for understanding in simplification, calling into question the representative complexity paradigm that has dominated climate model development.

Code and data availability The ECHAM-HAMMOZ model is freely available to the scientific community under the HAMMOZ Software License Agreement, which defines the conditions under which the model can be used. The specific version of the code used for this study is archived in the ECHAM-HAMMOZ SVN repository at /root/echam6-hammoz/tags/papers/2023/Proske_et_al_2023_ACPD. More information can be found on the HAMMOZ website (https://redmine.hammoz.ethz.ch/projects/hammoz, last access: 22 November 2023). Analysis and plotting scripts are archived at https://doi.org/10.5281/zenodo.10171426 (Proske et al., 2023f). Generated data is archived at https://doi.org/10.5281/zenodo.10184958 and https://doi.org/10.5281/zenodo.10183962 (Proske et al., 2023d; Proske et al., 2023e).

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5

Conclusions and outlook

5.1 Summary and conclusions

The starting point for this work is the detailed representation of aerosol and cloud microphysics that has accumulated in the global aerosol climate model ECHAM-HAM. The scheme complexity hinders model understanding, which is why we set out to find simplifications for the cloud microphysics and aerosol representation. Simplified models are easier to apply and perform sensitivity tests with since they enable time savings and are easier to manipulate. Besides, fewer components, processes or parameters ease understanding of the remaining model parts. Importantly, as we demonstrate, the process of developing simplifications already generates understanding of model behaviour.

For CMPs, we approached the quest for simplification bottom-up. In Chapter 2 we developed a methodology in which we perturb the effect that single processes have on the model state. Running many model variants with differently perturbed processes, we created a perturbed parameter ensemble (PPE). From the PPE, we built a surrogate model that allowed us to generate an even greater number of model simulations, which enabled us to perform quantitative sensitivity analysis on the PPE. Chapter 2 applies this methodology to four selected CMP processes. It demonstrates that this methodology can help us to, on the one hand, identify processes that the model is sensitive to. The model performance may benefit from improvements in these processes' representation. On the other hand the methodology enables us to identify processes that the model is not sensitive to. These processes are the ones that could be simplified or even completely neglected.

Chapter 3 applies the methodology to the whole CMP scheme, perturbing 15 processes. We identified 8 processes that the model is insensitive to and that thus could be simplified. Furthermore, we proposed and tested simplifications that set these processes' effects either to a constant value or to a climatology. Importantly, we found that the simplifications that we derived hold in past and future climates.

Thus, the simplified model remains useful for climate model applications of simulating different climate states.

In Chapter 4 we have turned towards a more drastic, top-down approach. We are interested in the behaviour of clouds in the model. The aerosol module provides input to the CMPs in the form of CCN and INP concentrations. In order to simplify the aerosol treatment, we have thus developed a climatological treatment of this interface. The climatologies either supply potential CCN and INP concentrations, which serve as input to the Lin & Leaitch cloud droplet activation scheme, or prescribe aerosol mass and number concentrations, which can enter both the Lin & Leaitch as well as the Abdul-Razzak & Ghan activation schemes. Overall, both climatologies give satisfying results in terms of cloud variables. One exception is in the Southern Ocean, where we find that CDNC concentrations are underestimated with a mean CCN climatology. Our investigation shows that the CCN climatology needs to include some treatment of aerosol hygroscopic growth in order to alleviate this bias. The other exception is an overestimation of CDNC in the Northern Hemisphere with the aerosol climatology using the Abdul-Razzak & Ghan activation scheme, which remains open for further investigation. Since they replace the whole HAM scheme, these simplifications enable large computational time savings.

Together, the chapters demonstrate that there is ample room for simplification in the aerosol and cloud microphysics treatment in ECHAM-HAM. This can be taken as evidence of redundancy in model formulations. Hence our work questions the approach of the representative vision, which seeks to “meet complexity in nature with model complexity” and where “redundancy in model detail is assumed to be a very long way off” (Shackley et al., 1998). Our approach adds to a range of recent work that studies model sensitivities and process simplifications and thus systematically questions model complexity (Cox et al., 2006; Crout et al., 2009; Gibbons et al., 2010; Tarsitano et al., 2011; Crout et al., 2014; Hieronymus et al., 2022). This work provides a new perspective onto model development: it calls to caution against the practiced call for greater model detail in response to model shortcomings. Instead, one may question whether new or more detailed parameterizations are really needed for one’s modeling purpose. Studying the model at hand may provide more efficient ways to improve a model’s adequacy for its purpose than simply adding more and more detail. At the very least, implementing new parameterization schemes should go hand in hand with comprehensive parameter sensitivity testing (Smalley et al., 2022).

Of course, for any given model the results of such simplifications depend on the model setup and scheme choice (White et al., 2017). On the first glance, this may seem to render our results less useful. In fact, the model employed in this study, ECHAM, is in the process of being replaced by its successor ICON (Zängl et al., 2015; Salzmann et al., 2022). However, ICON shares ECHAM dependencies. Most importantly, the value of our results lies not in exactly quantified model sensitivities, but rather in the broad-ranging conceptual implications, as detailed above and below. Thus they will remain valuable also in future model versions. In particular, the move to higher resolution modeling renders the processes that still need to be parameterized, such as aerosols and CMPs, even more important (Sullivan et al., 2022). Here the conclusion from our study remains valuable: climate model schemes contain redundancies and have room for simplifications that can enable us to understand the models better.

One outcome of our work is to expose the conflict between the representative and heuristic modeling visions. The representative vision assumes greater representational depth will make better models (and e.g. help to reduce uncertainty), while the heuristic vision uses models to generate understanding (see Sec. 1.3.2). Foremost, our work aimed at enhanced model understanding and thus served the heuristic vision. Importantly for the predictive vision, the results of our simplified model versions stay satisfyingly equifinal in global scale cloud variables. Thus the simplifications do no harm from the perspective of the predictive vision. However, the readiness to simplify is strongly related to the balance between the heuristic and representative visions. We question the expansive modeling paradigm that has historically dominated climate model development (see Fig. 1.2) and is deeply engrained in our modeling culture (see Sec. 1.2.3).

We demonstrate how the process of developing simplifications already helps in generating understanding of model behaviour. In this process, the model points the developer to which features are important. This gives a different perspective with much potential for model development and scientific insight. As Crout et al. (2014) state, in simplification "the aim should not be to simply find a simpler model and use it, but to use the identification of redundant variables as a means to challenge and improve the formulation used in the model." The new perspective, seeing what does and does not work in a simplified version, triggers a chain of checks and reasoning that is at the very root of the scientific methodology. This work demonstrates this power of simplifications to provide understanding of model behaviour: In Chapter 2 we found that ice crystal autoconversion dominates model sensitivities. This is troubling since the representation of ice crystal autoconversion may be seen as a violation of the physical representation ideal that is central to the idea of parameterizations (see Sec. 1.1.2). It is artificial in the sense that division between the categories of snow flakes and ice crystals exists only in the model. Thus, the sensitivity study has pointed us to a model behaviour that is unintended. Similarly, in the extensive CMP scheme study in Chapter 3, we found that the model is insensitive to some processes like the heterogeneous freezing of ice crystals or secondary ice production, while these processes are thought to be important for ice production in the atmosphere (see Sec. 3.3.4). Finally, the climatology that we derive for the Lin & Leaitch cloud droplet activation scheme only gave satisfying results for CDNC in the Southern Ocean when taking hygroscopic growth at cloud base conditions into account. With a simple mean climatology of CCN the CDNC was underestimated in the Southern Ocean. This implies that the naive replacement of the aerosol scheme with a purely observational CCN concentration is not viable. It requires online hygroscopic growth treatment (as in AEROclim), highlighting the critical role of that process.

5.2 Outlook

Fittingly, the points where we have derived understanding offer avenues for future work:

- **Large importance of ice crystal autoconversion** – As detailed in Chapter 2 and above, the large sensitivity of the model to this artificial process is troubling. It highlights that due to the "balance of approximations" (Lambert and Boer, 2001; Parker, 2009) and non-linearities, unphysical parts of the model may exert a disproportionally large influence. For ice crystal autoconversion the P3 CMP scheme offers relief. However, the tuning factor for ice crystal autoconversion which uses and exacerbates the processes' role in the model, is not the only "minor-looking treatment" (Kawai et al., 2022) in the model. Future sensitivity studies looking at other tuning factors, thresholds and alike could quantify their impact. As Hieronymus et al. (2022) suspect, "artificial parameters [...] might render some artificial assumptions more influential than the precise model physics." This quantification of their impact could in turn help to hedge model uncertainties as well as guide model development. For such a study, our PPE and sensitivity analysis method could be readily employed.

- **Unimportance of some CMP processes** – In Chapter 3 we have shown that heterogeneous freezing and secondary ice production have a negligible impact on global cloud variables in ECHAM-HAM, which goes against experimental understanding. Unless they dramatically enhance these processes' effectiveness, new parameterization formulations will not help to alleviate this problem. Our hypothesis is that other processes in the model dominate the balance of processes. For example, heterogeneous freezing of cloud droplets is thought to be important as a threshold process that supplies the first ice crystals that are needed to initiate a cloud phase transition. Our hypothesis is that in the model the sedimentation of ice crystals from above already supplies those crystals, rendering heterogeneous freezing unimportant. This hypothesis has been and is being explored in a number of projects (Chadzelek, 2023; Ickes et al., 2023a). In particular, the question of which processes drive ice crystal number concentrations in ECHAM-HAM will be explored in the FOR-ICE (Ickes et al., 2023b) project. In this model intercomparison project, switches for all processes that can supply ice crystals to the model, are being implemented. Running the model for all possible combinations of switches allows to use the factorial method (Montgomery, 2017), which attributes the importance of each process for ICNC, similarly to our approach in Chapter 2 and 3.

- **Aerosol climatology** – We have explained the SO bias in CDNC to stem from a missing consideration of hygroscopic growth at high humidity cloud conditions with the mean climatology. The aerosol climatology similarly leads to an overestimation of CDNC in the Northern Hemisphere when using the AR&G activation scheme. We propose a similar investigation of possible processes or feedbacks leading to that behaviour as we conducted for the SO bias in Sec. 4.3.3. Since the Northern Hemisphere bias is smaller with the L&L scheme, here the problem likely lies not in the prescribed CCN concentrations themselves but rather in the interaction with the AR&G activation scheme.

- **Observation based CCN climatology** – The code developments we have implemented for Chapter 4 open up the possibility to use an observation-based CCN climatology instead of the model-derived one. Our results highlight that some treatment of hygroscopic growth is required, so any mean climatology would require adaptions. The use of an observation-based climatology would also only be possible for climate states for which observations exist, limiting its usefulness for the study of climate change. However, at least for present day simulations, supplying an observation-based CCN climatology is an avenue to lead out of the complexity paradigm created by the combination of reductionism and representative goals.

- **Evaluate simplified model variants** – We have constructed various sets of simplified model variants and have evaluated their performance in past and future climates both for the CMP process representations in Chapter 3 and for the climatological simplifications in Chapter 4. For the latter, a thorough investigation of model state and important climate change metrics such as the equilibrium climate sensitivity will be conducted as part of the FORCeS project. The CCN/INclim-cloudbase model variant will take part in the FORCeS intercomparison. For this, we perform historical and time-evolution simulations, both with the default full HAM setup and the simplified model version. With other models that will perform the same set of simulations these will form the basis for extended evaluations.

A

Assessing the potential for simplification in global climate model cloud microphysics

A.1 Tuning

Table A.1: Tuning parameters that differ between this study and the reference of Neubauer et al. (2019). γ_r is the scaling factor for the stratiform rain formation rate by autoconversion. γ_s is a scaling factor for the stratiform snow formation rate by autoconversion. With the changes described in Sec. 2.2.1 the tuning parameter of the maximum cloud droplet radius, r_{CDNC}, replaces the previous minimum cloud droplet number concentration, $\mathrm{CDNC}_{\mathrm{min}}$. The tuning parameter for immediate autoconversion of detrained ICNC, γ_d, is newly introduced.

Parameter	ECHAM-HAM this study	Reference
γ_r	5	10.6
γ_s	600	900
r_{CDNC}	$15 \times 10^{-6}\,\mathrm{m}$	–
$\mathrm{CDNC}_{\mathrm{min}}$	–	$40 \times 10^{-6}\,\mathrm{m}^{-3}$
γ_d	5	–

A.2 PPE results for more variables

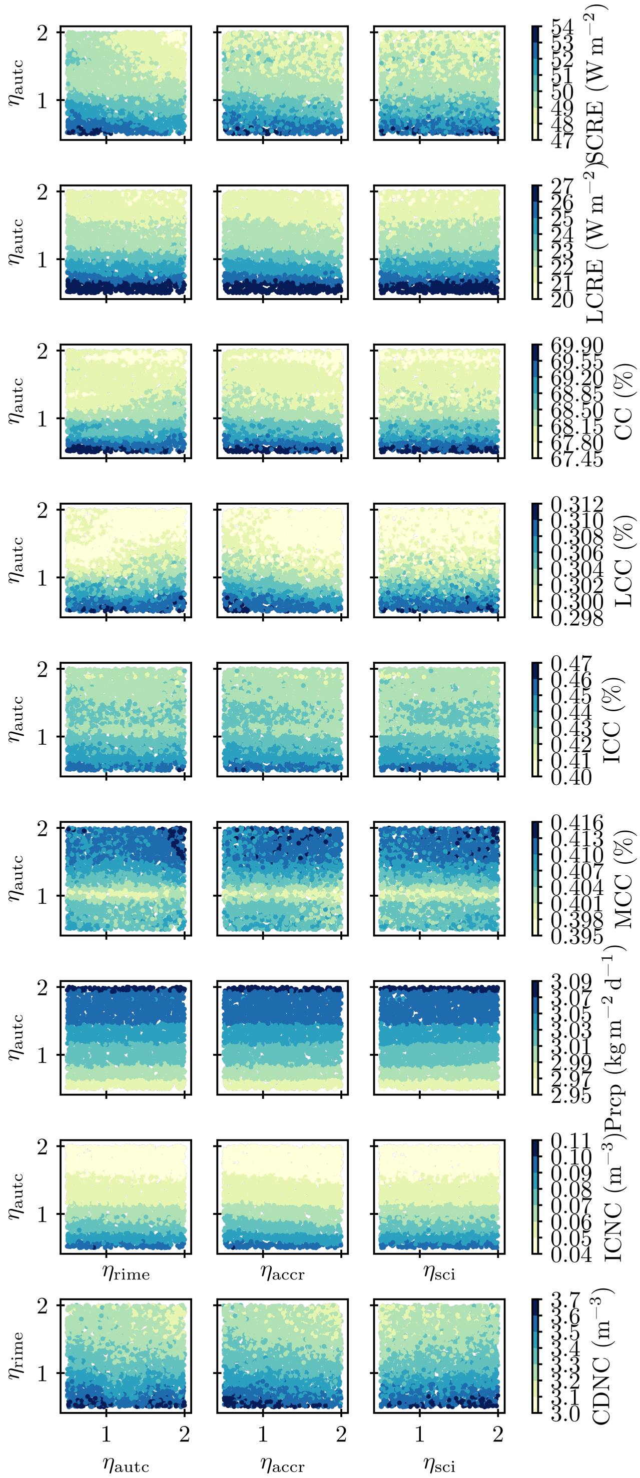

Figure A.1: Visualisation of the multi-dimensional response surfaces of the emulated PPEs for multiple variables. Each process is a dimension, and the colorbars denote the global annual mean values. In principle, each surface could be displayed by a full matrix plot as in Fig. 2.7 and 2.8, but here only the panels that include the dominating process are shown (autoconversion, except for CDNC in the last row, where riming is the dominant process).

A.3 Total sensitivity index

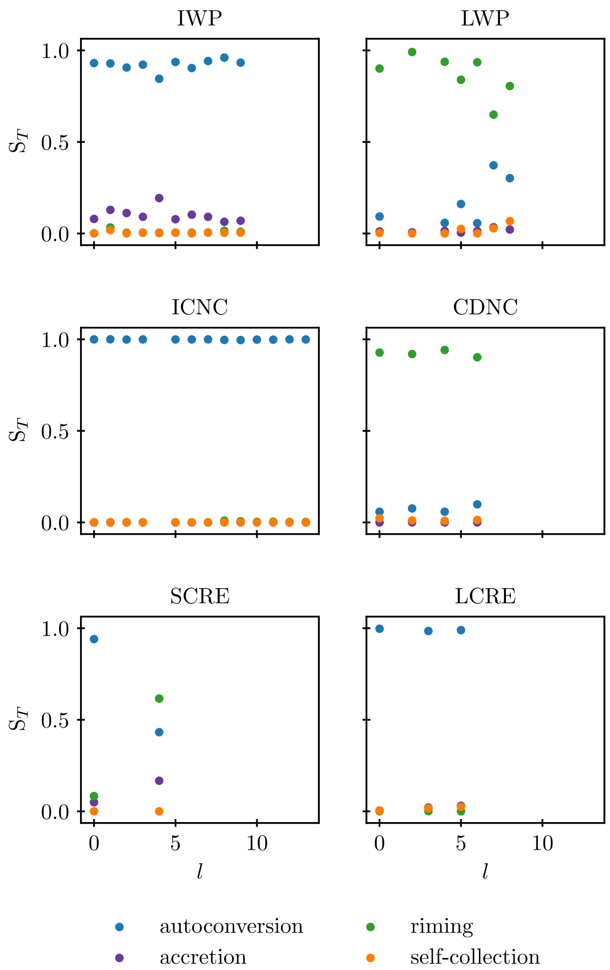

Figure A.2: Same as Fig. 2.11 but for the total sensitivity indices.

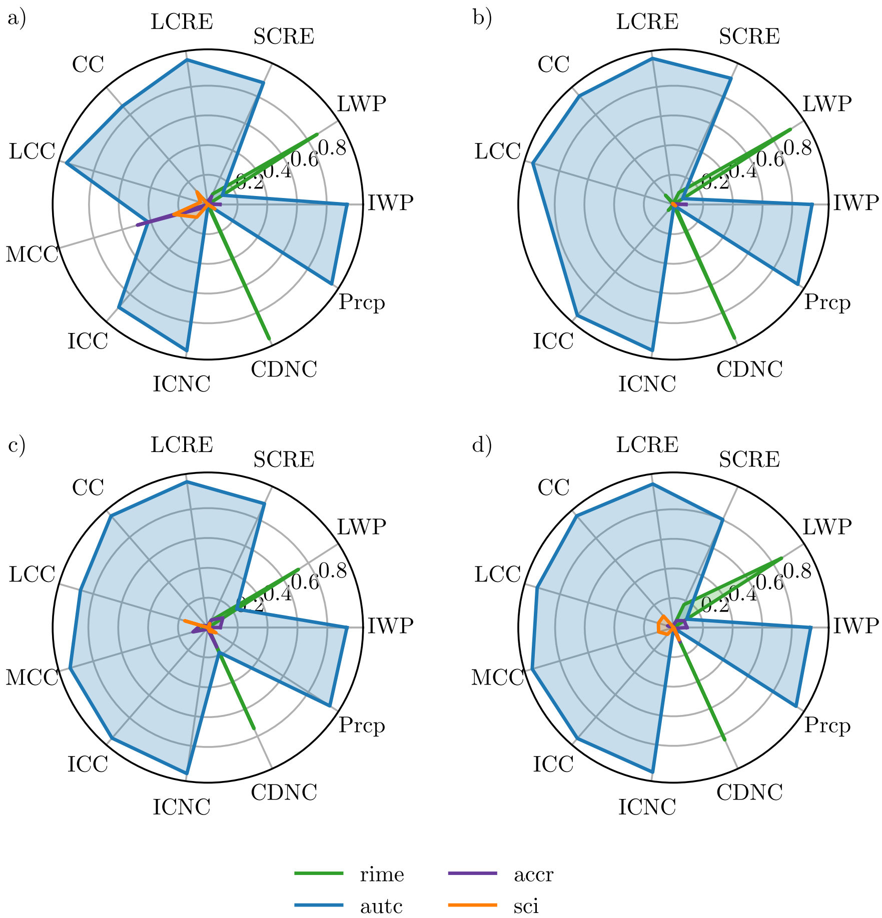

Figure A.3: Same as Fig. 2.12 but for the total sensitivity indices.

A.4 Validation of the spherical harmonics sensitivity analysis

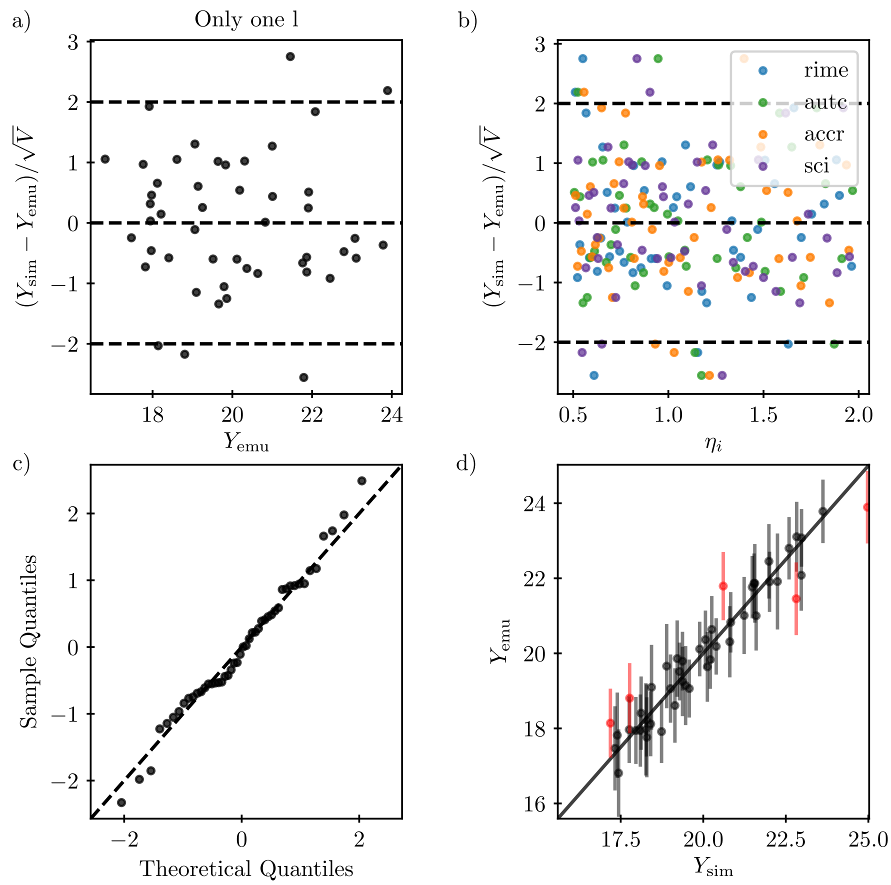

Figure A.4: Validation of the emulated angular amplitude spectrum of degree $l = 6$ for the LWP.

The validation of the spherical harmonics emulation was carried out as described in Sec. 2.2.4. Larger uncertainties in the emulation were apparent for almost all variables and degrees l (see Fig. A.4 for an example) than for that of the global mean values. However, some emulations were also found to be defaulting, meaning that they predicted a similar output value for the whole phase space (see Fig. A.5 and A.6 for an example). As this behaviour points to a missing signal in the input, these points were excluded from further analysis, if the following two criteria were not fulfilled (excluding the emulated outliers that are marked red e.g. in Fig. 2.4):

- The uncertainty in the prediction is smaller than the spread of the variable, i.e. the smallest error bar in Fig. A.4d) is smaller than $0.9\Delta Y_{\mathrm{sim}}$.
- The predictions are significantly different from each other, i.e. there is one pair of predictions whose error bars do not overlap.

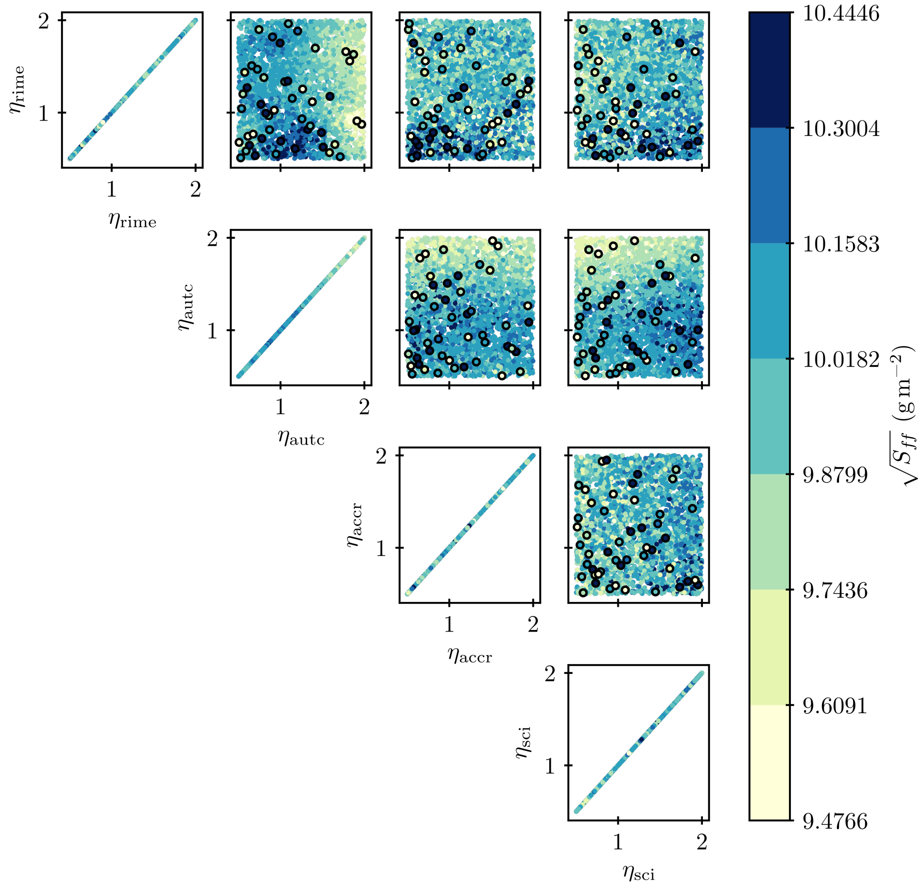

Figure A.5: Same as Fig. 2.7 but for the LWP spherical expansion angular amplitude spectrum of degree $l = 3$. In this case, the emulator was found to be defaulting and therefore failed the validation and was not included in the subsequent sensitivity analysis. The points enclosed by black circles denote the PPE member results used to train the emulator.

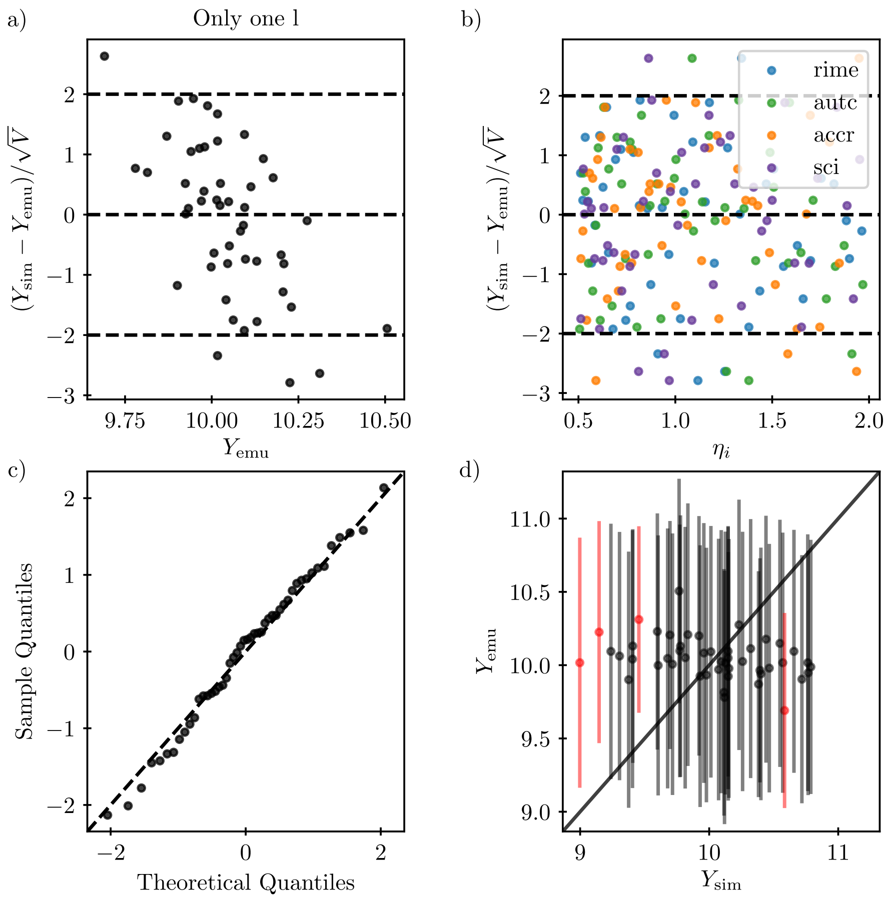

Figure A.6: Validation of the emulated angular amplitude spectrum of degree $l = 3$ for the LWP (see Fig. A.5), which failed because of diagnosed defaulting.

B

Addressing complexity in global aerosol climate model cloud microphysics

B.1 Tuning

Table B.1: Tuning parameters for the P3 scheme that differ between this study and the reference of Dietlicher et al. (2019). γ_r is the scaling factor for the stratiform rain formation rate by autoconversion. γ_{sci} is the scaling factor for the self-collection of ice. For the 2M scheme the tuning was the same as described in Table A.1.

Parameter	ECHAM-HAM (P3) this study	Reference
γ_r	3.25	8
γ_{sci}	7	5

B.2 Simplifications: climatologies

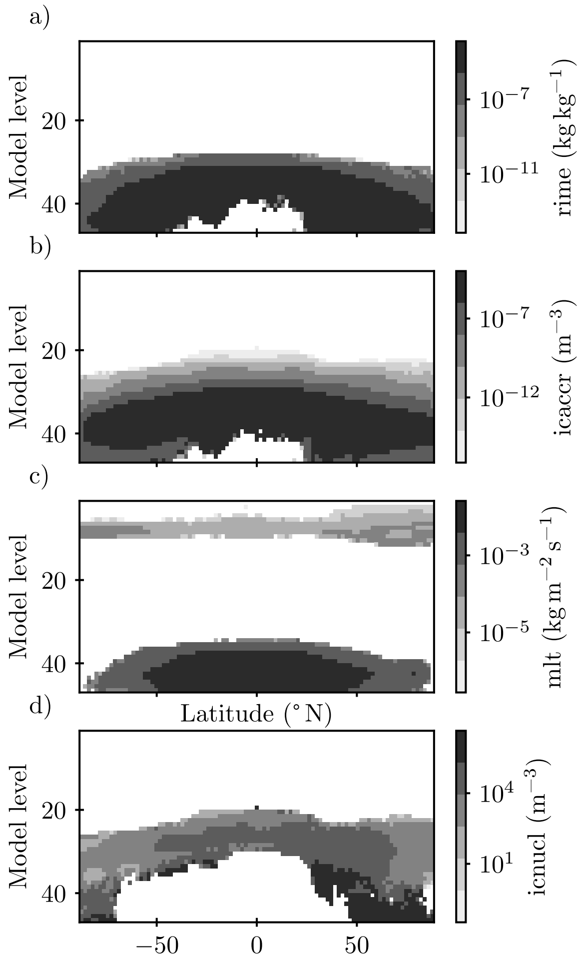

Figure B.1: Zonal mean climatologies that were prescribed for the simplification experiments for **(a)** riming, **(b)** ice crystal accretion, **(c)** melting, and **(d)** ice crystal nucleation.

B.3 Total sensitivity indices

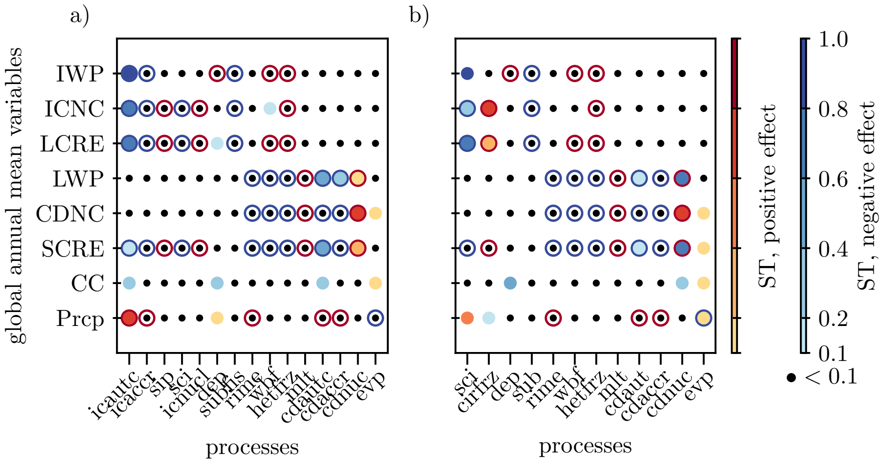

Figure B.2: As Fig. 3.7 but for the total sensitivity indices.

C

Developing a climatological simplification of aerosols to enter the cloud microphysics of a global climate model

C.1 Tuning

Table C.1: Tuning parameters for the L&L scheme that differ with respect to the ECHAM-HAM model version used in Chapters 2 and 3 (see Tables A.1 and B.1). The latter's tuning is used for the AR&G scheme. γ_r is the scaling factor for the stratiform rain formation rate by autoconversion. γ_s is a scaling factor for the stratiform snow formation rate by autoconversion.

Parameter	L&L this study	Reference and AR&G this study
γ_r	3.25	5
γ_s	900	600

C.2 Sensitivity simulations to elucidate the SO-bias

To understand the SO-bias in CDNC exhibited by CCN/INclim-mean (see Sec. 4.3.3), we conducted various sensitivity simulations:

- **Aerosol species emissions** – The SO aerosol composition is dominated by sea salt and sulfate, where in the Northern Hemisphere dust and black or brown carbon are more important. Sea salt and DMS emissions (with DMS being a precursor for sulfate) are highly dependent on wind speed, which might

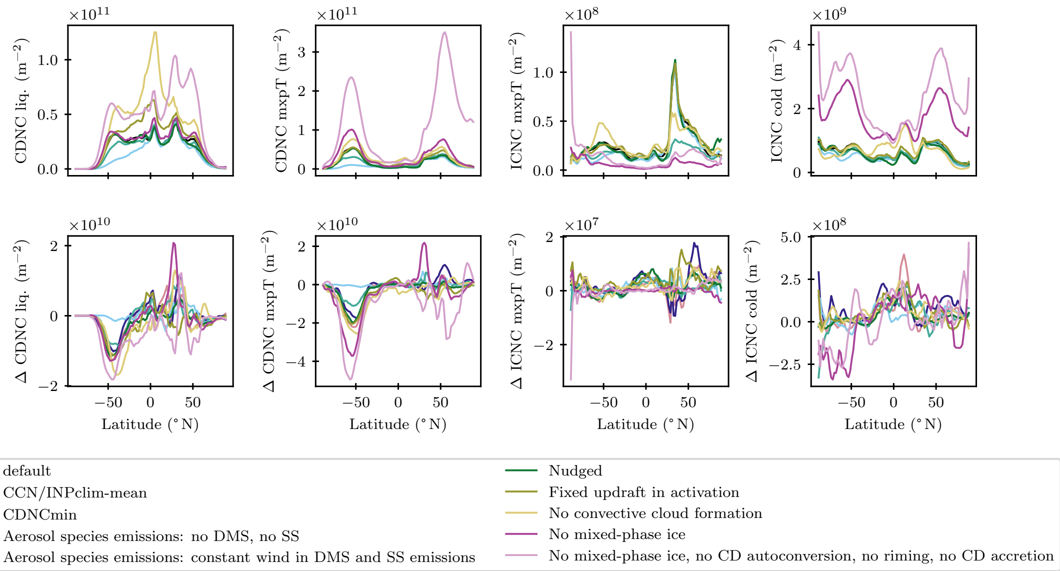

Figure C.1: As Fig. 4.4, but for sensitivity simulations with different ways to create the CCN/INPclim-mean climatology. Differences are shown relative to the respective default simulations (indicated by the colors). Only the default mean climatology and the one created using only CCN values higher than the CDNC minimum are shown as differences to the default simulation (shown in black). Dimethyl sulfide (DMS) is a precursor of sulfate aerosols, SS stands for sea salt and CD for cloud droplet. For the "no mixed-phase ice" simulations, heterogeneous cloud droplet freezing as well as ice crystal sedimentation were inhibited.

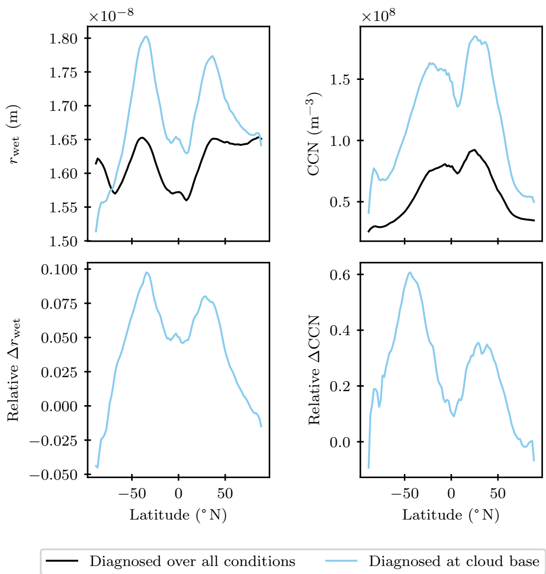

Figure C.2: Zonal mean of vertically averaged wet radii and CCN, diagnosed from all conditions and only at cloud base. The second row shows the zonal mean of the vertically averaged differences.

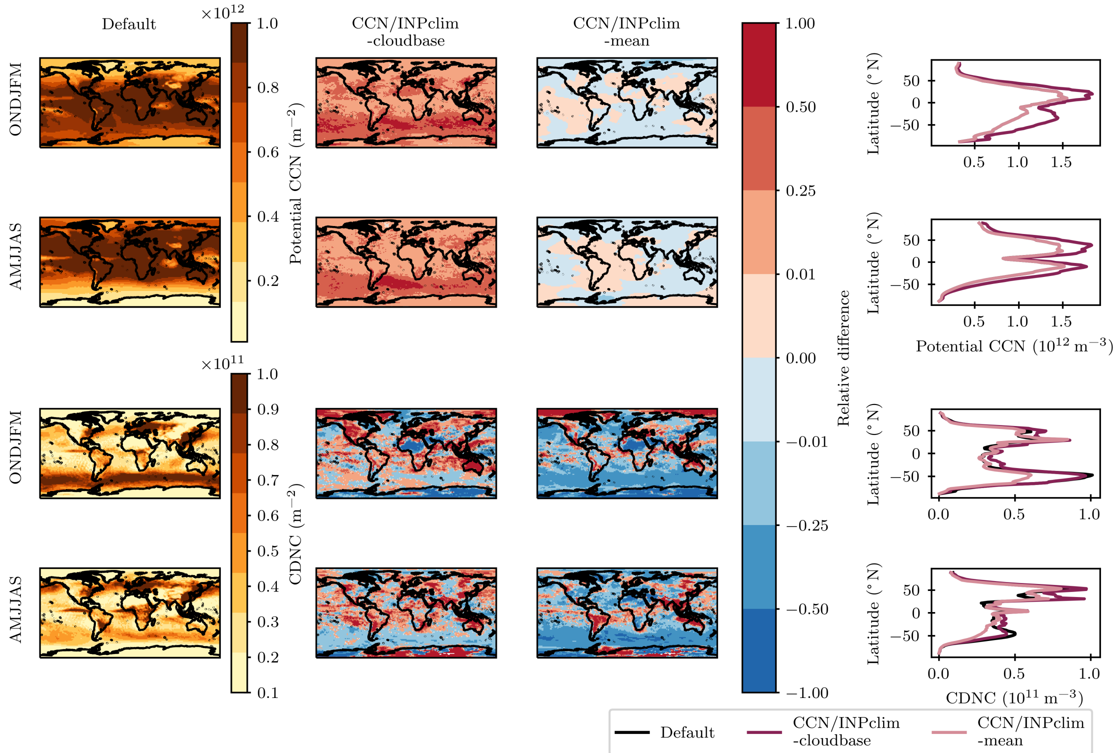

Figure C.3: Seasonal mean maps of potential stratiform CCN concentrations (top two rows) and CDNC concentrations (bottom two rows), in absolute terms for the default simulation (left most column) and relative deviations for the different climatologies. The right most column shows the absolute zonal means. Note that for potential CCN, the default is hidden behind the CCN/INPclim-mean line.

lead to high variability, making the climatological representation less suited for the SO. We tested this hypothesis by prescribing a fixed wind speed in the emission computations. This approach changes the default CDNC as expected, but the bias in the SO remains. As an extreme test, we turned off DMS and sea salt emissions separately (not shown) and together. This reduces CDNC both in the default and the CCN/INPclim-mean case. Turning off both DMS and SS, the difference between the full HAM and climatology simulation in the SO disappears, but CDNC are small in the full HAM simulation to begin with. Turning both emission types off separately does nothing to alleviate the SO bias.

- **Nudging** – By nudging pressure, vorticity and divergence we can test whether feedbacks from the cloud behaviour to the dynamics of the model are contributing to the discrepancy. Since the SO discrepancy remains in the nudged case, we can exclude these types of feedbacks as a reason for it.

- **CDNCmin** – To avoid unphysical situations, climate model code employs thresholds and other "minor-looking treatments" (Kawai et al., 2022). One of these is the CDNC minimum that serves to avoid situations where the model calculates a cloud with too few, too large cloud droplets. In our ECHAM-HAM configuration, the minimum is calculated dynamically from the in-cloud water content and a set droplet radius (see Sec. 2.2.1). CCN concentrations below the CDNC minimum threshold value are never effective in promoting cloud droplet formation. However, they do enter into the CCN/INPclim climatology and may thus artificially lower effective values. We tested the effect of this threshold for the CCN climatology by allowing only CCN larger than the minimum to enter the climatology. Since the sensitivity simulation preserves the SO bias we can exclude CDNCmin as the reason for the SO discrepancy.

- **Fixed updraft** – As illustrated in Fig. 4.2, both the potential CCN and the local updraft enter the calculation of activated cloud droplets. This updraft could be affected by dynamical feedbacks to a CCN perturbation. Thus we conducted simulations where we put the value of the updraft that is used in the activation calculation to a constant value. This of course deteriorates the performance in the default simulation, but since it does not reduce the SO bias from CCN/INPclim-mean, we can exclude the updraft hypothesis as well.

- **Convective cloud formation** – The CCN/INPclim prescribes CCN not only for stratiform but also for convective clouds. Cloud droplets that formed in convective clouds may enter stratiform clouds by detrainment. To test the effect of detrainment we inhibited convective cloud formation. This of course changes the default simulation, but again it does little to reduce the SO CDNC bias.

- **Mixed-phase ice phase influence** – In the SO we expect different cloud phase distributions and cloud properties than in the Northern Hemisphere (Mülmenstädt et al., 2015), with e.g. lower ice crystal number concentrations in the SO (see Fig. 4.4). The difference in cloud phases could explain differing reactions of the clouds to changes in CCN and cloud droplet formation. We tested this hypothesis in a simulation where all mixed-phase clouds were forced to remain liquid by inhibiting heterogeneous cloud droplet freezing as well as ice crystal sedimentation. The resulting simulations show neither a better CCN/INPclim-mean performance in the SO in terms of CDNC, nor a worse performance in the Northern Hemisphere. Hence we can exclude the ice phase as a reason for the SO discrepancy.

- **CMPs processes** – Other CMPs processes might lead to feedbacks that enhance the CDNC discrepancy in the SO. We tested this hypothesis by turning off both the ice phase influence (as above), and the processes of cloud droplet autoconversion, riming and cloud droplet accretion. Hence in this simulation all processes leading to liquid precipitation formation or influencing cloud droplet number concentrations (except nucleation) were inhibited (see Fig. 3.2). Removing the CDNC sink processes greatly enhances CDNC as expected. However, the underestimation of CDNC in the SO by CCN/INPclim-mean remains.

C.3 Simplification performance in different climate states (PD, PI and FUT simulations)

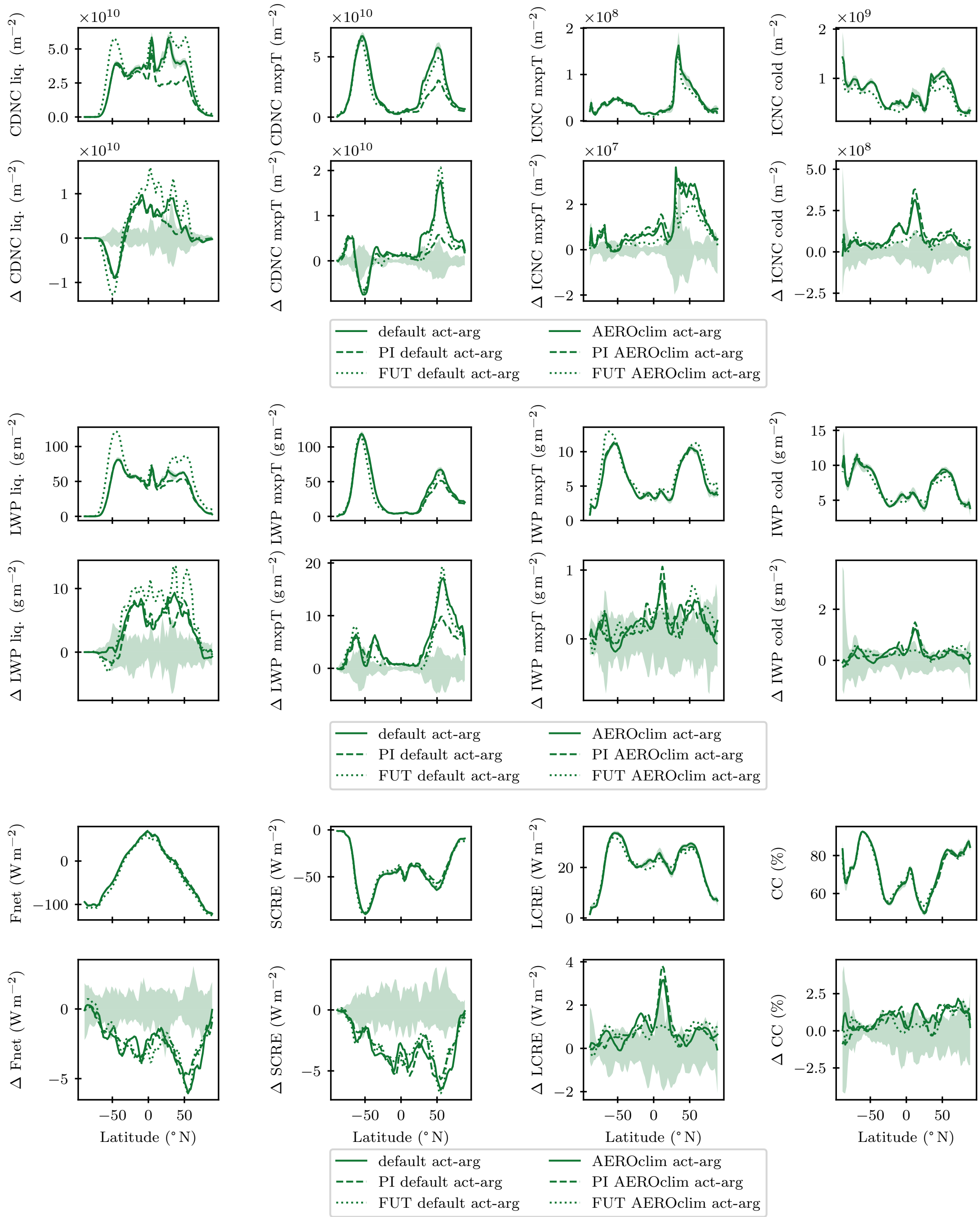

Figure C.4: As Fig. 4.7, but for the act-arg scheme default and AEROclim simulations.

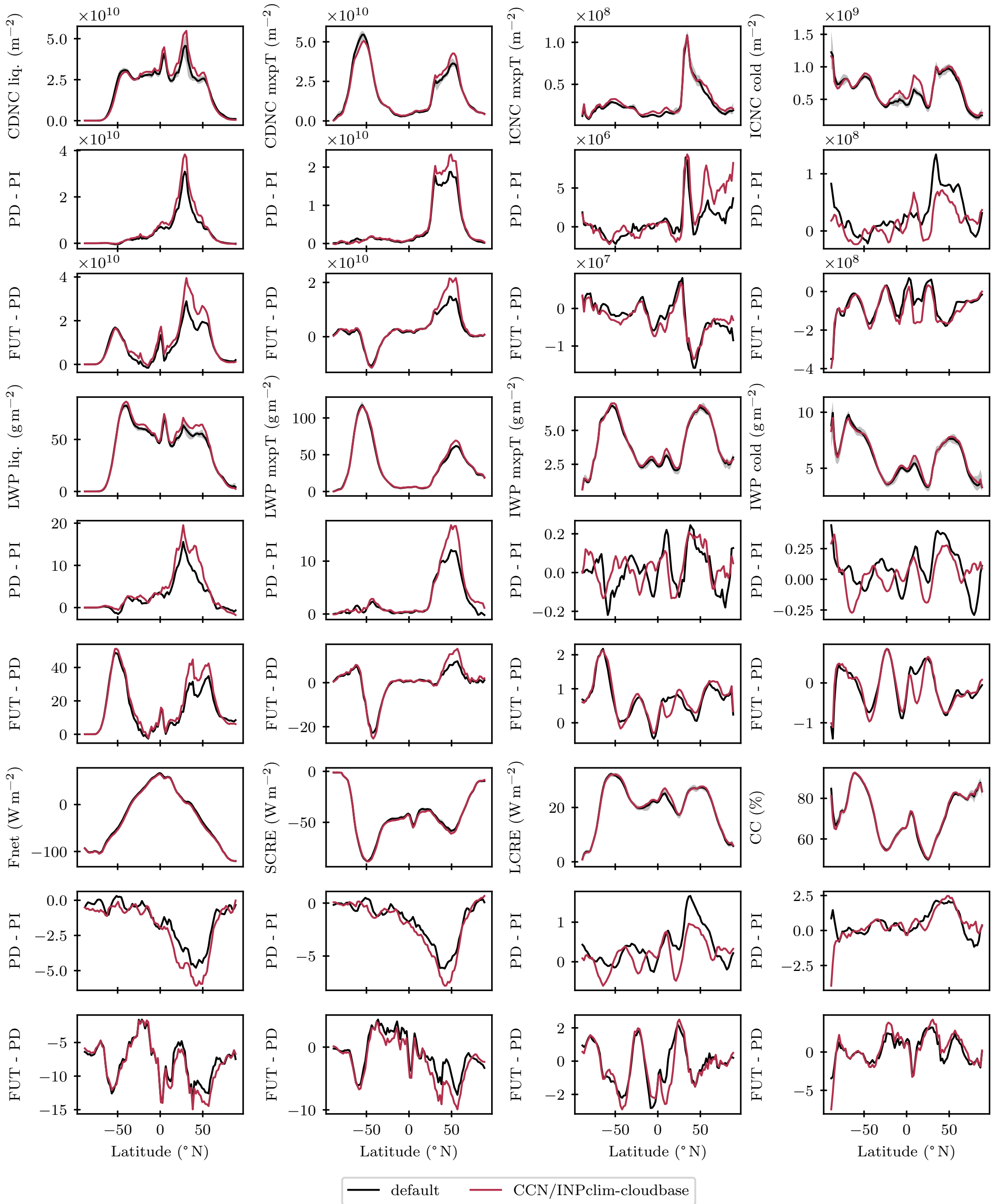

Figure C.5: As Fig. 4.7, but comparing the aerosol radiative forcing and difference between SST + 4 K and present conditions (as described in Sec. 4.2.2) between the default and CCN/INclim-cloudbase simulations.

D Acronyms

CC cloud cover

CCN cloud condensation nuclei

CDNC cloud droplet number concentration

CMP cloud microphysical

CMPs cloud microphysics

ICNC ice crystal number concentration

IWP ice water path

LCRE longwave cloud radiative effect

LWP liquid water path

PPE perturbed parameter ensemble

Prcp precipitation

$\mathbf{S}_1$ first direct effect sensitivity index

$\mathbf{S}_\mathrm{T}$ total effect sensitivity index

SCRE shortwave cloud radiative effect

SO Southern Ocean

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