Systematic Correlation Matrix Evaluation (SCoMaE) - A bottom-up, natural science-based approach to identify Indicators

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Abstract. This study introduces the Systematic Correlation Matrix Evaluation (SCoMaE) method, a bottom-up approach which combines expert judgment and statistical information to systematically select transparent, non redundant indicators for a comprehensive assessment of the state of the Earth system. The methods consists of three basic steps: 1) Calculation of a correlation matrix among variables relevant for a given research question, 2) Systematic evaluation of the matrix, to identify clusters of

5   variables with similar behavior and respective mutually independent indicators, and 3) Interpretation of the identified clusters, enabling a learning effect from the selection of indicators. Optional further analysis steps include: 4) Testing the robustness of identified clusters with respect to changes in forcing or boundary conditions, 5) Enabling a comparative assessment of varying scenarios by constructing and evaluating a common correlation matrix, or 6) Inclusion of expert judgment such as to prescribe indicators, to allow for considerations other than statistical consistency. The exemplary application of the SCoMaE method

10   to Earth system model output forced by different CO_2 emission scenarios reveals the necessity of re-evaluating indicators identified in a historical scenario simulation for an accurate assessment of an intermediate-high, as well as a business-as-usual, climate change scenario simulation, which arises from changes in prevailing correlations in the Earth system under varying climate forcing. For a comparative assessment of the three climate change scenarios, we construct and evaluate a common correlation matrix, in which we identify robust correlations between variables across the three considered scenarios.

15   # 1 Introduction

An indicator is a quantitative value, measured or calculated, that describes relevant aspects of the state of a defined system. A useful indicator should fulfill certain characteristics that depend on the purpose of the indicator (Gallopín, 1996). Environmental indicators are developed based on quantitative measurements or statistics of environmental conditions in order to allow for a comparison of states of the environment across time or space (Ebert and Welsch, 2004). For environmental indicators of

20   climate change Radermacher (2005) defined statistical measurability, political and societal relevance and scientific consistency, i.e. a scientifically meaningful link between indicator and the state to be described, as three main characteristics that should be considered as important during the indicator selection process. Moreover, other characteristics can be defined as desirable for such indicators, such as a high signal-to-noise ratio of the measurement, the relevance for ethical considerations, or the fact that the chosen indicators should not provide redundant information.

For the assessment of ongoing climate change, models representing the physical and biogeochemical processes of the Earth system, so called Earth system models (ESMs), are one of the essential tools, because the inertia of the climate system to (carbon) perturbations requires projections of future climate states. Early climate models applied simple zero to two dimensional calculations to assess the effect of atmospheric CO_2 on the climate by using global mean surface air temperature (SAT) as an indicator (e.g., Arrhenius, 1896; Callendar, 1938; Sellers, 1969). This commonly used climate change indicator, SAT, fulfills all three above mentioned characteristics: Several long term temperature records as well as proxies for assessing SAT exist, which makes this indicator well measured (Statistical measurability). SAT is closely linked to other climate variables, e.g. evaporation, sea level rise, or biological productivity. Although SAT may not be the most relevant variable for society, using this indicator as a proxy for climate impacts is scientifically consistent (Seneviratne et al., 2016). Its political, economical and ethical relevance evolved over time and is now evident in discussions concerning e.g. global warming (Ott et al., 2004) or the 2-degree temperature increase target, which was endorsed by the Conference of the Parties in 2015 (UNFCCC, 2015).

As Earth system models continuously increase in complexity there are more and more output variables available that could potentially serve as indicators for the state of the climate system. Which ones should we regard for a comprehensive assessment, ideally, without providing redundant information? A common bottom-up approach for measuring such complex systems is to start from a broad set of (Earth system) variables and consecutively select more appropriate ones depending on the research question (e.g. Pintér et al. (2005); Kopfmüller et al. (2012)). For natural science-based climate change assessments reports, such as published by Working Group I of the Intergovernmental Panel on Climate Change (IPCC), the task of selecting scientifically consistent indicators to inform policy and the general public is a highly non-trivial task. In addition to SAT, nowadays many additional indicators are selected to evaluate changes in different components of the Earth system, e.g., precipitation, or often precipitation extremes, the Arctic summer sea ice or the rate of ocean acidification etc. As such they are discussed in e.g. the IPCC's summary for policy makers of the recent assessment report of climate change (Stocker et al., 2013).

However, given a certain data set, already the selection of an indicator is a normative choice and there exist no unambiguous rules for the selection process (Krellenberg et al. (2010) and Böhringer and Jochem (2007), respectively). Any selection process of indicators and construction process of metrics from Earth system variables implies a value and weighting decision, applying a weight of zero on any disregarded variable. While the value judgment ideally requires the inclusion of potential end-users or stakeholders, the weighting requires a well-informed and broad participation of scientific disciplines, i.e., expert judgment (Radermacher, 2005).

In this study we go beyond the usual scientific approach of applying expert judgment to select indicators for addressing a given research hypothesis, and introduce a bottom-up method that combines expert judgment with statistical information on the data set to systematically select scientifically consistent indicators. Systematic Correlation Matrix Evaluation (SCoMaE) uses information on correlations between variables to identify "clusters" of variables that show similar behavior, and hence can be represented by one key indicator. The identified indicators are independent and do not provide redundant information. A set of independent indicators hence allows for a more comprehensive natural science-based assessment of the system under consideration than a set of correlated indicators. Furthermore, SCoMaE allows for a learning process by providing new information about correlations between the given variables, and hence can help to increase the process understanding.

To illustrate the SCoMaE method, we apply it to the output of an Earth system model of intermediate complexity, the University of Victoria Earth system climate model (UVic ESCM). We select indicators from Earth system variables for a comprehensive assessment of our simulated climate system, given three forcing scenarios, namely a historical scenario, an intermediate high CO_2 emission scenario, and a business as usual emission scenarios (see Appendix A). This example enables us to 1) illustrate how a correlation matrix can be constructed given a specific research question, 2) identify a comprehensive indicator set for the historical forcing scenario, 3) show that an indicator set derived from a historical forcing scenario is not necessarily appropriate to describe future states of the climate system under global warming, 4) identify a common indicator set valid for all three forcing scenarios, and finally 5) illustrate how the method could be used in an iterative process including expert judgment or previous knowledge of the given system. These steps will serve as the guideline of this paper.

2   The Systematic Correlation Matrix Evaluation (SCoMaE) method

2.1   Step 1: Calculate the Correlation Matrix

Throughout this study, a variable is defined as a model output or observational time series, whereas we refer to it as an indicator if a variable was selected to represent a certain aspect of the considered system. To obtain a comprehensive, non redundant set of indicators to describe a given system, the first step is to construct a correlation matrix, i.e. a matrix including the correlation information of all the relevant Earth system variables to each other. The construction of the correlation matrix strongly depends on the research question and needs to be adjusted accordingly. The selection of which variables are the relevant variables for the given research question and hence should be included in the matrix, as well as the choice on how the correlations should be calculated is very important for the outcome of the study. Correlations could for example be calculated between time series of variables or their derivatives, absolute temporal changes, or spatial patterns. Alternatively, output from ensemble simulations could be used to calculate correlations between variables. The matrix is then evaluated based on the significance information of these correlations (see Step 2).

To illustrate the construction of the matrix based on our example simulations we show how the correlation between global mean 'surface air temperature' (A_sat) and 'northern hemisphere sea ice area' (O_iceareaN) in the Representative Concentration Pathway (RCP) 8.5 emission scenario (Meinshausen et al., 2011) translates to the corresponding correlation matrix entry (Figure 1). In our example we want to study the correlations between model output variables, given their reaction to varying model input parameters concerning poorly constrained parameter processes in the model impacting the simulated carbon cycle. Assuming that the signal of interest is of a similar kind as the state differences between the start and the end of a climate change simulation, we start by calculating the temporal differences between 2005–2015 and 2090–2100 from a number of parameter perturbation simulations that serve as our ensemble in this example (see Appendix B for explanations of the parameter perturbations). This enables us to learn whether the different output variables show a similar behavior for the respective parameter perturbation. Then the correlation between these changes are calculated and tested by performing a two sided test on a 5% significance level, with $N = 16$, the number of perturbed parameter simulations, and accordingly $t_{crit} = 2.145$.
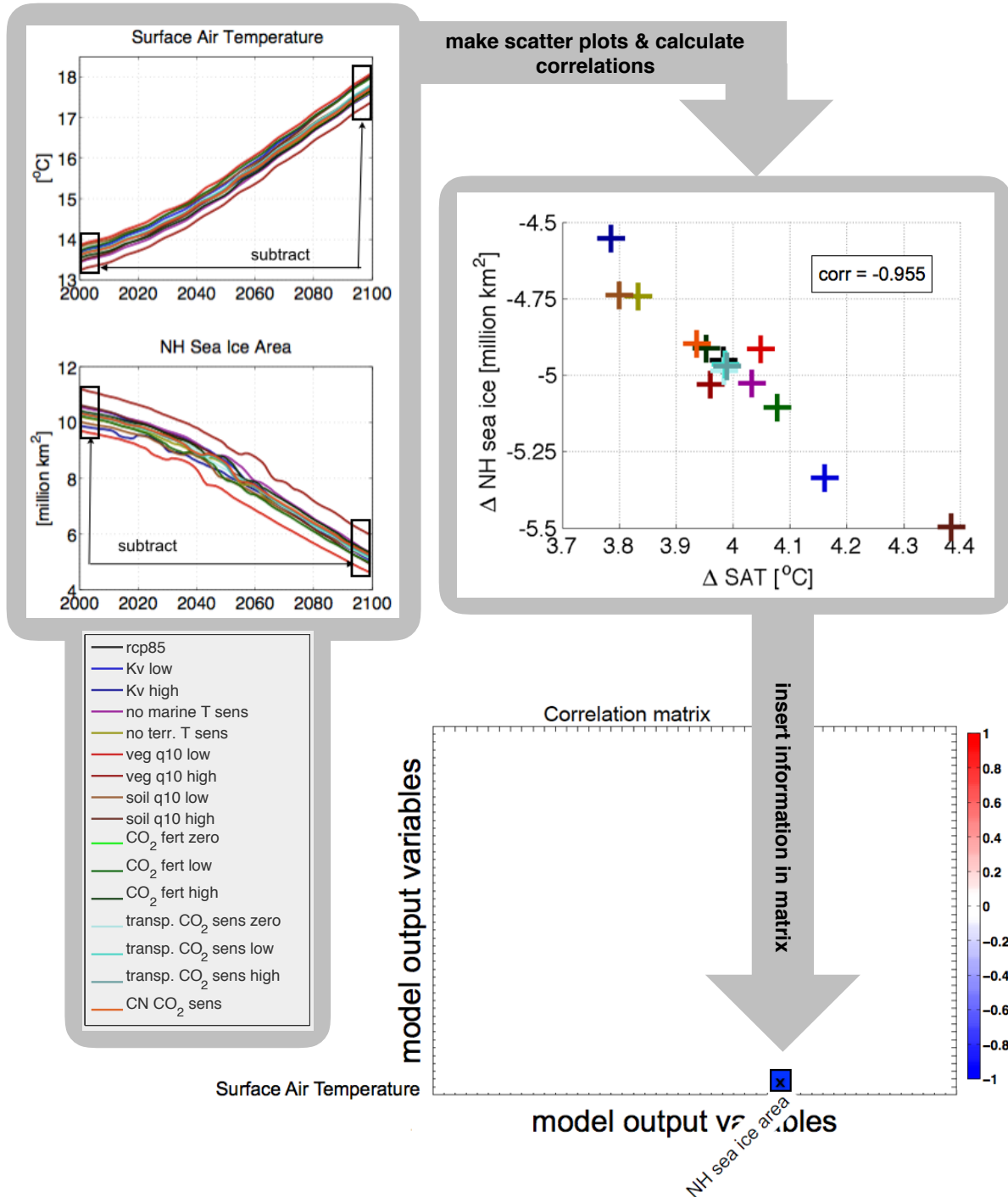
Figure 1. Illustration of the Correlation Matrix Construction for the example of surface air temperature (SAT) and northern hemisphere (NH) sea ice area. Temporal differences of the simulations are calculated between 2005-2015 and 2090-2100. These are then correlated and this information is used for the entry in the correlation matrix.

In our example, there is a negative correlation evident between temporal changes in 'surface air temperature' (A_sat) and 'northern hemisphere sea ice area' (O_iceareaN). This illustrates that these model output variables show opposite reactions towards the parameter perturbations, i.e. if the perturbation causes surface air temperatures to increase, it also causes northern hemispheric sea ice to decrease. This information is then written into the correlation matrix. By studying the constructed correlation matrix (see Figure 3), and studying single correlations between model output variables, we can learn about basic correlations within the simulated climate system, and test if these agree with our expectations. To simplify the visual analysis of our example we sorted the variables in the matrices according to their strength in correlation towards the commonly used climate change indicator surface air temperature, A_sat in our model, in the historical scenario.

2.2 Step 2: Cluster identification and indicator selection

To obtain a set of indicators for the assessment of changes in the regarded system, we systematically evaluate the previously constructed correlation matrix (see Figure 2 for an illustration of this procedure). To obtain a comprehensive, non-redundant indicator set, we follow these steps: 1) The first indicator is the variable with the highest number of significant correlations towards other variables. 2) All variables with a significant correlation are clustered under this indicator. 3) These clustered variables are then excluded from the selection of the next indicator. 4) The next indicators is again the variable with the highest number of significant correlations towards all the remaining variables. 5) This indicator selection procedure is repeated until all variables are clustered and are represented by an indicator. If a variable is not significantly correlated to any of the remaining variables, this variable is considered to be a single indicator. These single indicators are needed for a fully comprehensive assessment, since they show a different behavior from all previously selected indicators and hence provide additional information.

In our example we applied this procedure to the correlation matrix of the historical forcing scenario as simulated by the UVic ESCM (See Appendix A for details on the simulations). We find that the first indicator is precipitation over ocean areas (F_precipO) (Figure 3 and S5). By following the respective column of F_precipO (17th from the right) in the correlation matrix we can see that this model output variable is significantly correlated to all variables that are also significantly correlated to A_sat (1st from the bottom), with the exception of 'mean ocean temperature' (O_temp, 16th from the bottom),but in addition also links global and terrestrial precipitation and evapotranspiration (F_precip/L and F_evap/L, respectively, and 35th and 37th from the bottom) as well as the 'surface net upward longwave radiation' (F_uplwr, 40th from the bottom). These variables are not significantly correlated to 'surface air temperature' (A_sat). Hence based on purely statistical considerations using 'precipitation over ocean' (F_precipO) as an indicator for the historical period, would be preferable to global mean 'surface air temperature' (A_sat), the main indicator for historical climate change, since it potentially holds more information.

'Surface albedo on land' (A_albsurL) is identified as the second indicator. It is, after excluding all variables correlated to 'precipitation over ocean' (F_precipO), significantly correlated to 'net surface downward shortwave radiation' (F_dnswr), 'ocean oxygen' (O_o2) and 'sea surface salinity' (O_salsur). The third indicator is 'ocean surface alkalinity' (O_alksur), which shows the same response to the parameter perturbations as 'ocean surface phosphate concentrations' (O_po4sur). When excluding all
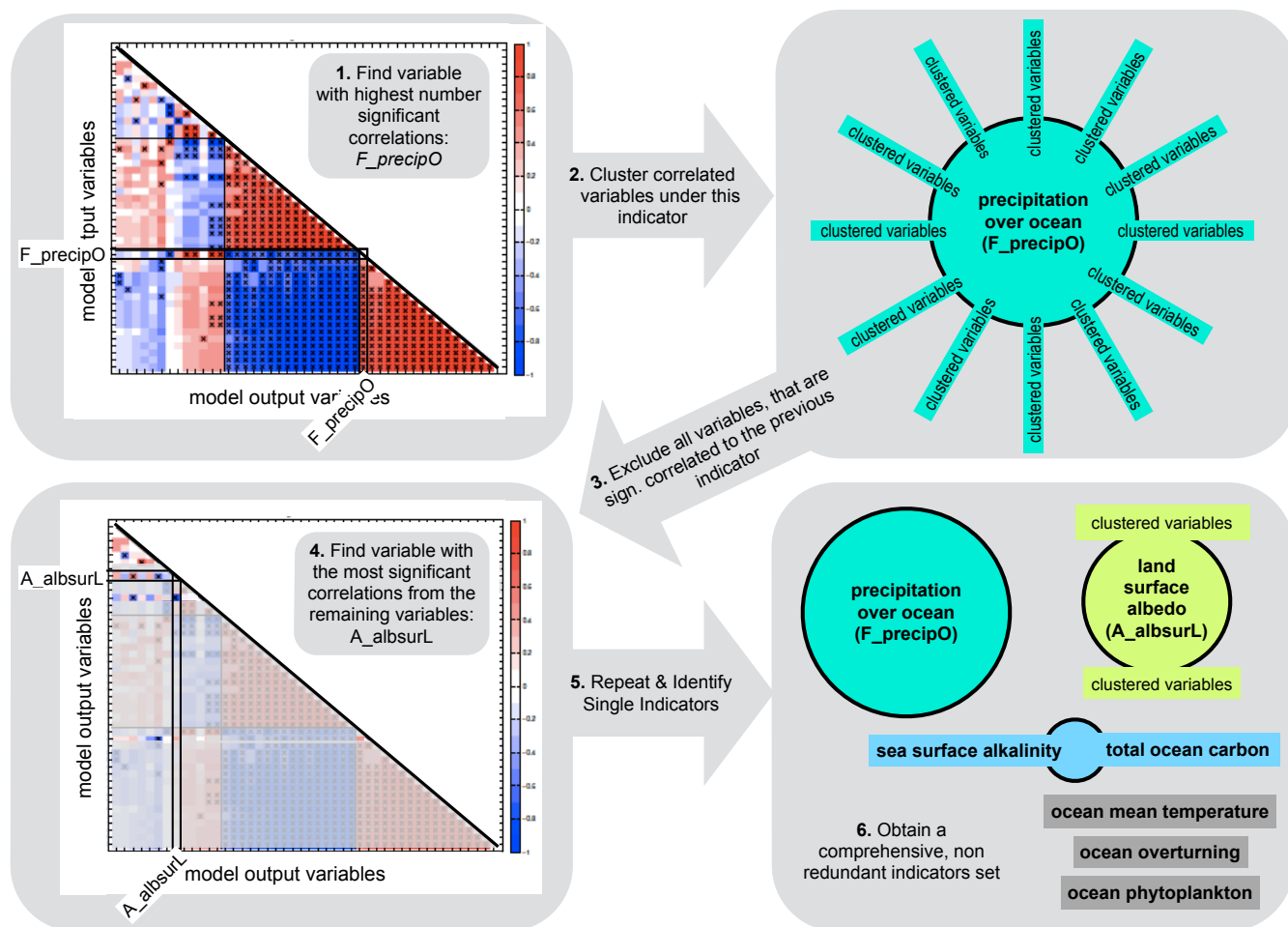
Figure 2. Illustration of the indicator selection process on the example of the correlation matrix for the historical scenario. See Section 2.2 for a detailed step-by-step description of the evaluation process.

variables that are correlated to either one of the three above mentioned indicators, three variables remain unclustered: 'Mean ocean temperature' (O_temp), 'maximum meridional overturning' (O_motmax), and 'ocean phytoplankton' (O_phyt). These variables are hence single indicators, which are needed for a comprehensive assessment of the system under consideration (Figure 3b).

5 (See Section 1 and Figures S1 and S2 in the supplementary material, for the results of these analyses for the intermediate-high (RCP4.5) and the business as usual (RCP8.5) scenarios, respectively.)
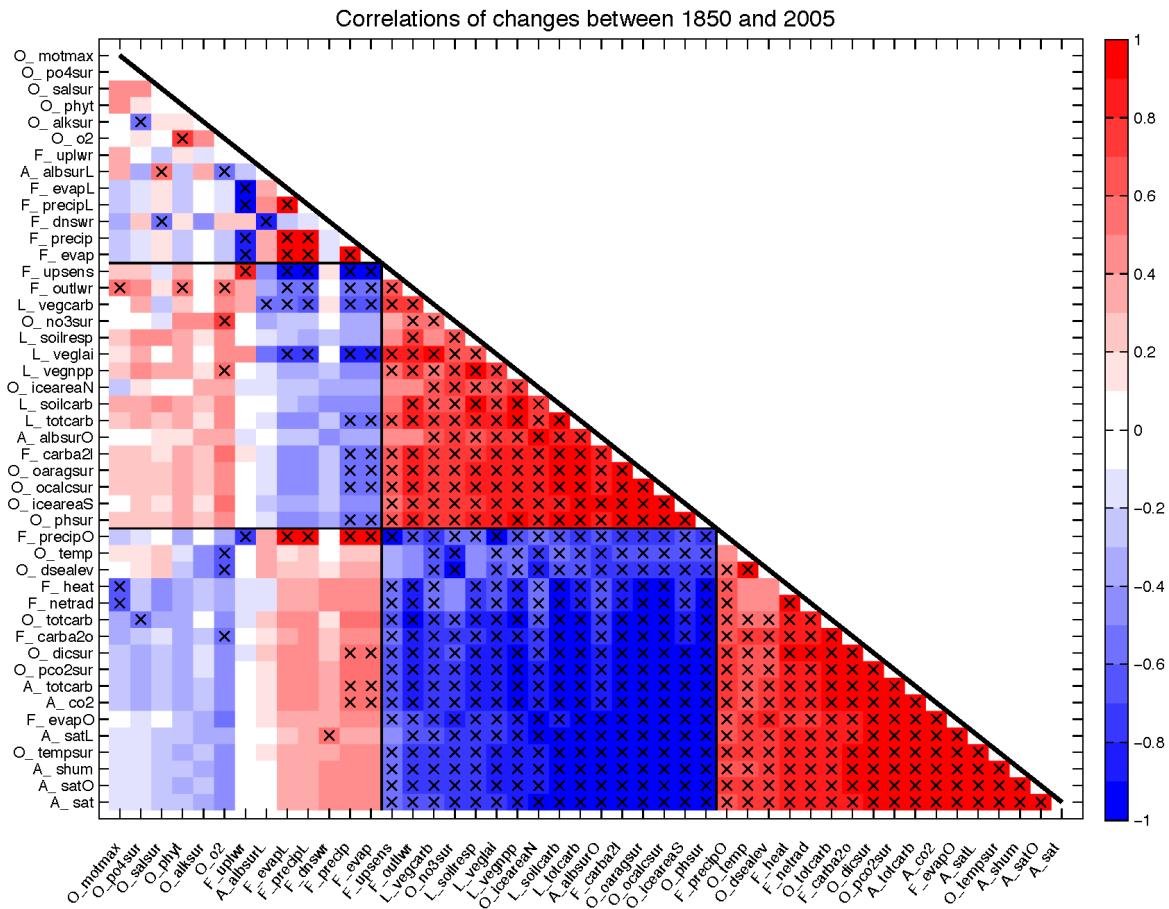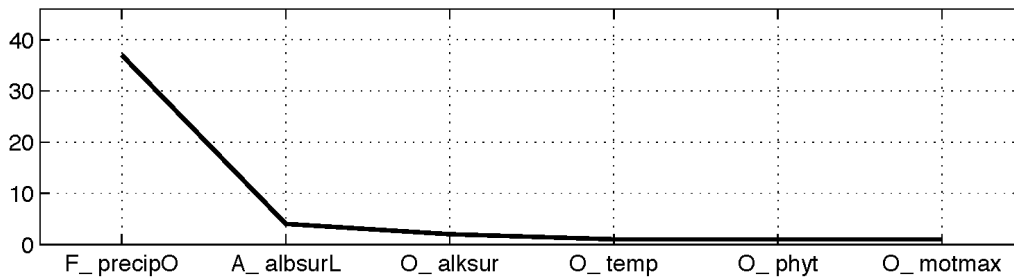
Figure 3. top: Correlation matrix for the historical simulation scenario. The correlations are calculated according to the example of Figure 1 from the results of the perturbed parameter simulations for each of the 46 model output variables, respectively. Correlations significant on a 5% significance level are marked with 'x'. The order of the variables was determined based on their correlation strength to surface air temperature (A_sat) in the historical scenario. For details on the regarded model output variables see Table S1.

bottom: Indicators as identified from our analysis based on the correlation matrix above as illustrated in Figure 2, ranked by the amount of significant correlations.

2.3 Step 3 (optional): Comparison of indicators for the different forcing scenarios

In order to learn how well the previously identified indicators for one scenario explain a different scenario with changed forcing, we prescribe the use of the previously identified indicator set. The SCoMaE accordingly first uses these indicators and then analyses if and which additional indicators are needed for a fully comprehensive assessment of the new scenario.

For the example we prescribed the indicators identified for the historical scenario to assess the intermediate-high (RCP4.5) and the business as usual (RCP8.5) emission scenarios (Figure 4). The results show, that if we were to only utilize the indicators from the historical scenario for the assessment of the two RCP scenarios, we would not be able to assess all changes in the climate system as represented by our model: For the RCP4.5 scenario, we would obtain additional information by considering

10 the variables 'net top of atmosphere radiation' (F_netrad) and 'ocean surface heat flux' (F_heat), which are clustered together, and 'net upward longwave radiation' (F_uplwr) and 'ocean surface salinity' (O_salsur), which form another indicator cluster (Figure 4).

Note, that Earth system variables clustered under the prescribed indicators differ among the different scenarios (compare Figure 3 and S1): In the historical scenario the indicator 'precipitation over ocean' (F_precipO) includes the output variables 'net top

15 of atmosphere radiation' (F_netrad), 'ocean surface heat flux' (F_heat), 'ocean surface nitrate' (O_no3sur), 'top of atmosphere outgoing longwave radiation' (F_outlwr), and 'net upward longwave radiation' (F_uplwr), all of which are not included in the 'precipitation over ocean' (F_precipO) indicator for the RCP4.5 scenario. Instead, the indicator 'precipitation over ocean' (F_precipO) for the RCP4.5 scenario includes 'mean ocean temperature' (O_temp), which it is not included for the historical scenario.

20 The differences between the correlation matrices for the RCP8.5 scenario compared to the historical scenario are even larger (compare Figure 3 and S2). For the RCP 8.5 scenario eight out of 46 considered variables would not be included if we applied the indicators identified for the historical scenario. Instead we need three additional indicators for the assessment of the system under consideration, namely 'net top of atmosphere radiation' (F_netrad), 'ocean surface dissolved inorganic carbon' (O_dicsur), and 'net surface downward shortwave radiation' (F_dnswr) (Figure 4). Note that six of the eight remaining vari-

25 ables that were initially included in the first indicator cluster for the historical scenario, namely 'precipitation over ocean' (F_precipO), are no longer significantly correlated to it for the RCP8.5 scenario.

These differences in the correlation matrices for the different forcing scenarios indicate changes in prevailing correlations between Earth system variables with climate state. This illustrates that it a reevaluation of the chosen indicators may be needed for a comprehensive assessment of different climate strategies yielding different climate states.

30 2.4 Step 4 (optional): Evaluation of a common correlation matrix

To advance this analysis such that changes in correlation matrices from different forcing scenarios can be taken into account, it is possible to create a correlation matrix representing only those correlations that are significant in all forcing scenarios, a so-called common correlation matrix. Applying the SCoMaE method to such a common correlation matrix identifies an indicator
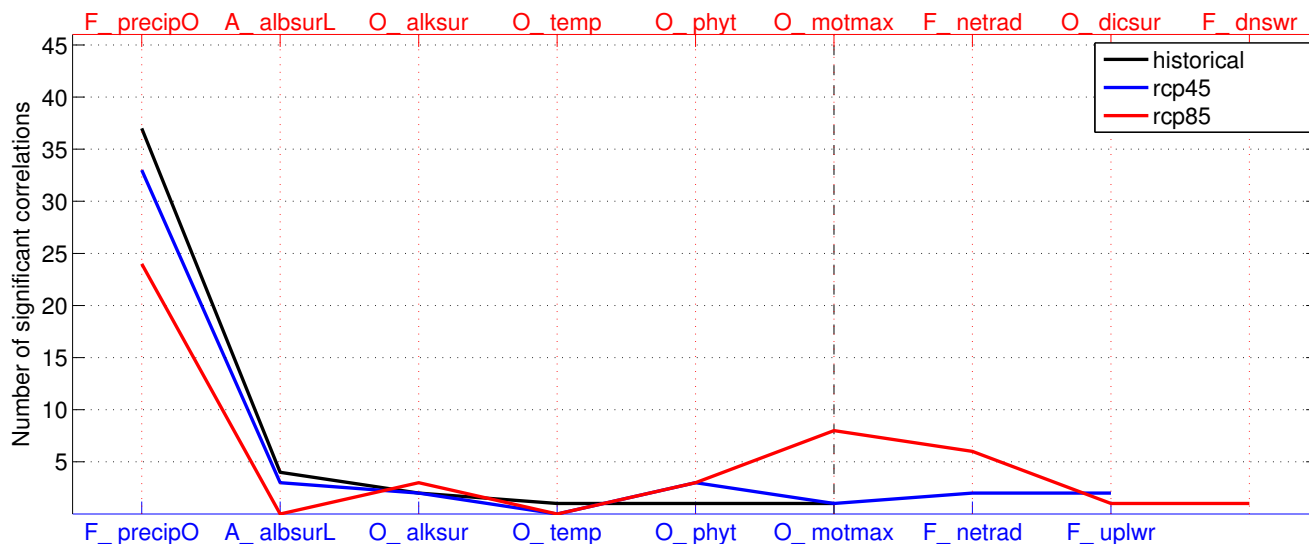
Figure 4. Indicators identified from the analysis of the RCP4.5 (blue) and RCP8.5 (red) correlation matrices with the precondition to use the historical indicators first.

set that can be used to assess and also compare multiple scenarios, and hence differs from the previously identified sets for the individual correlation matrices.

To obtain a common indicator set for the three exemplary forcing scenarios (historical, RCP4.5 and RCP8.5), we construct
5   a correlation matrix in which only correlations that are significant in all these scenarios are considered (Figure 5). Furthermore the color shading indicates in which scenario the correlations were found to be significant.

A first visual evaluation of the common correlation matrix shows more reddish than bluish shading, which indicates that the correlation patterns for the historical and RCP4.5 scenarios are more similar, than for the historical and RCP8.5 scenarios (Figure 5). This means that for a lower future emission scenario, the indicators from the historical scenario are more suitable than
10   for a higher future emission scenario. This is true with the exception of the terrestrial and oceanic carbon fluxes (F_carba2l and F_carba2o, respectively), which are perturbed more by the land-use scheme implemented in the RCP4.5 scenario, since this scenario includes a high amount of afforestation and reforestation. Furthermore, greenish shading shows correlations that are significant only in the RCP scenarios, indicating that those correlations depend on the increasing anthropogenic (mainly CO_2) forcing, included only in these scenarios.
15   The first indicator obtained from the common SCoMaE analysis is 'atmospheric CO_2' (A_co2), which was also found to be the first indicator in the RCP8.5 scenario (Figures S7 and S8). It is significantly correlated to 27 other output variables in all three scenarios, indicating that these correlations are robust and independent of the different strength of CO_2 forcing in the different scenarios. The fact that 'atmospheric CO_2' (A_co2) is the first indicator with a large number of correlated variables, hints at
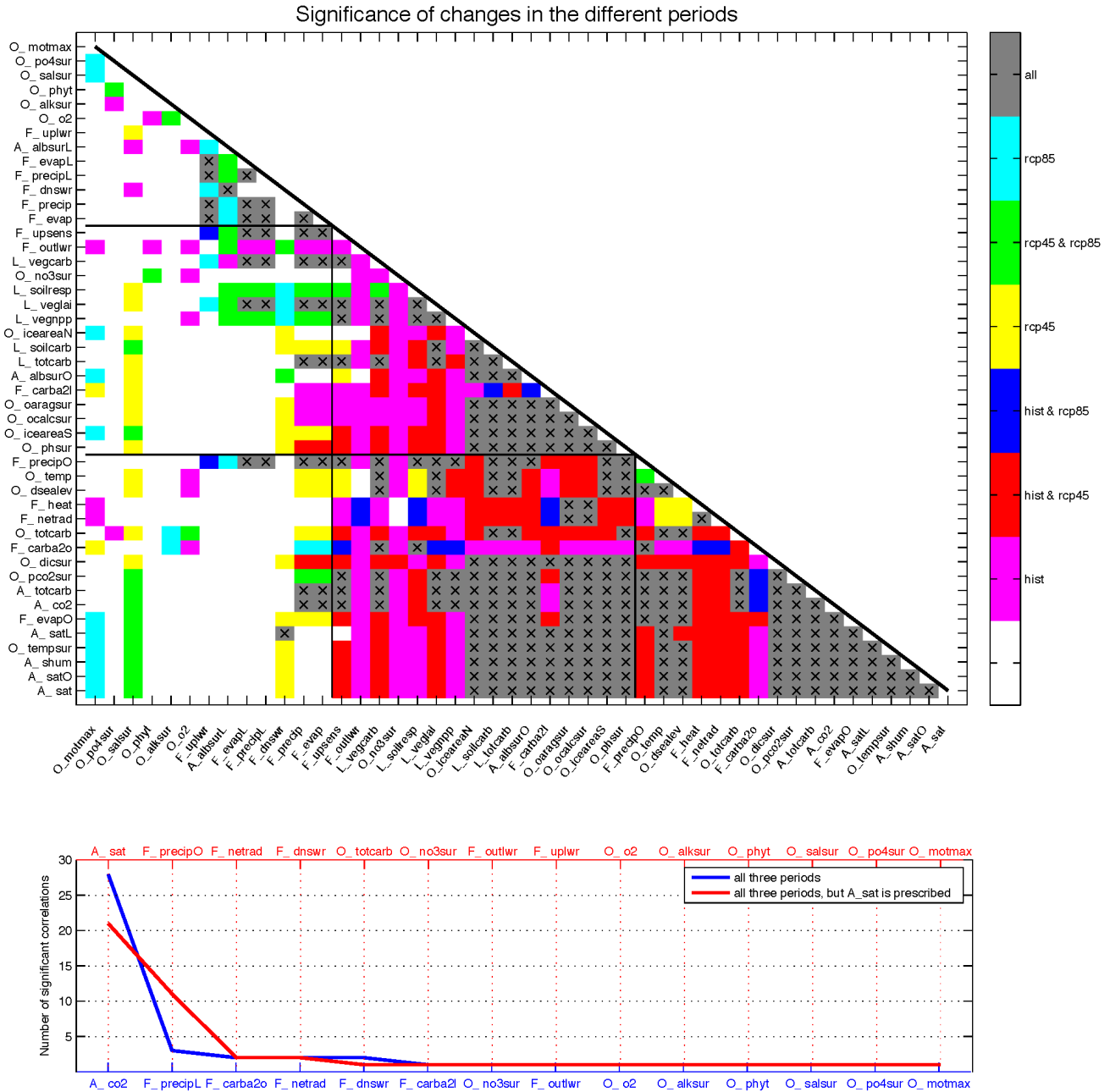
Figure 5. a) Correlation matrix for all three scenarios, the colors indicate in which scenarios the corresponding variables show a significant correlation, see colorbar for explanation. The 'x's mark combinations of variables, where the correlation is significant on a 5% significance level in all three scenarios. For details on the regarded model output variables see Table S1.

b) indicators as identified from the analysis based on the correlation matrix above against the number of significant correlations (blue) and with the condition, that surface air temperature (A_sat) is prescribed as the first indicator (red).

its importance in determining the reaction of other Earth system variables during climate change e.g. changes in temperatures, carbon fluxes and moisture fluxes over the ocean.

The second indicator is 'precipitation over land' (F_precipL), which is clustered with 'terrestrial evapotranspiration' (F_evapL) and 'net upward longwave radiation' (F_uplwr) (Figure S8). This cluster accordingly represents changes in terrestrial moisture

5 fluxes and the resulting surface upward fluxes of longwave radiation. The latter relates to the surface air temperature, which on land is strongly influenced by the amount of evapotranspiration, and the resulting evaporative cooling. Note, that the fact that terrestrial moisture fluxes are clustered under a separate indicator, hints at a different sensitivity of these variables to climate change and the perturbed parameters. Since these three variables show significant correlations to each other in all three scenarios, one could use any of them as the indicator for this cluster. The same is true for the next indicators and their clusters, which

10 are 'air to sea carbon flux' (F_carba2o) and 'soil respiration' (L_soilresp); 'net top of atmosphere radiation' (F_netrad) and the 'ocean surface heat flux' (F_heat); and 'net surface downward shortwave radiation' (F_dnswr) and the 'land surface albedo' (A_albsurL).

The remaining single indicators are 'air to land carbon flux' (F_carba2l), 'ocean surface nitrate' (O_no3sur), 'top of atmosphere outgoing longwave radiation' (F_outlwr), 'ocean oxygen' (O_o2), 'ocean surface alkalinity' (O_alksur), 'ocean phytoplankton'

15 (O_phyt), 'sea surface salinity' (O_salsur), 'ocean surface phosphate' (O_po4sur) and 'maximum ocean meridional overturning' (O_motmax).

2.5 Step 5 (optional): Including expert judgment

If stakeholders or experts were to inform the indicator selection process, it is possible to prescribe indicators and then use the

20 SCoMaE analysis to identify additional uncorrelated variables, that are needed to obtain a comprehensive assessment of the system. Also instead of using global mean time series, one could look at time series of regions or already processed variables, such as heat stress or cumulative emissions. This approach in combination with the SCoMaE analysis enables us to learn about variables, which have previously been disregarded but potentially provide new information about the system, or to learn which of the previously regarded indicators actually provide redundant information.

25

How would the common indicator set from our example change, if we were to include the condition that 'surface air temperature' should be the first indicator, instead of 'atmospheric CO_2'?

Prescribing 'surface air temperature' (A_sat) as the first indicator for the common correlation matrix, leads to the replacement of 'precipitation over land' (F_precipL) by 'precipitation over ocean' (F_precipO) as the second indicator (Figure 5,

30 bottom), which is correlated with 12 variables that are clustered under this indicator. Almost all of these variables were initially clustered under 'atmospheric CO_2' (A_co2), but are not significantly correlated to 'surface air temperature' (A_sat). These variables mainly describe global and oceanic moisture fluxes, as well as carbon fluxes or reservoirs on land: 'precipitation over the ocean' (F_precipO), 'global evaporation' (F_evap), 'global precipitation' (F_precip), 'vegetation net primary productivity' (L_vegnpp), 'leaf area index' (L_veglai), 'vegetation carbon' (L_vegcarb) and the 'surface upward sensible heat flux'

(F_upsens). The only exception to this behavior is 'total ocean carbon' (O_totcarb), which in turn becomes a single indicator. In addition the second indicator, 'precipitation over the ocean' (F_precipO), now incorporates the previously identified clusters of the second and third indicators, namely the clusters of 'precipitation over land' (F_precipL) and the 'air to sea carbon flux' (F_carba2o). Only 'net upward longwave radiation' (F_uplwr), which was also clustered under 'precipitation over land'

5   (F_precipL) becomes a single indicator, remaining unclustered when 'surface air temperature' (A_sat) is prescribed as the primary indicator. In turn 'air to land carbon flux' (F_carba2l), which was a single indicator in the default SCoMaE analysis, is now clustered under 'surface air temperature' (A_sat).

The third and fourth indicators are 'net top of atmosphere radiation' (F_netrad) and 'net surface downward shortwave radiation' (F_dnswr), which were found with the same underlying clusters in the default analysis (compare Figures S8 and S9). Finally,

10   eight of the nine previously identified single indicators, remain unclustered and hence are still single indicators.

Although the total number of indicators has not changed, the identified clusters and their meaning differ: In the default analysis the first indicator represented changes in temperatures, carbon fluxes and global and oceanic moisture fluxes. If 'surface air temperature' (A_sat) is prescribed the global and oceanic moisture fluxes are moved to the second cluster, which in addition incorporates some Earth system variables from the previously identified second and third indicators. This is one example showing

15   how the SCoMaE method allows for the inclusion of expert judgment or preconditions, is able to account for changes in correlation patterns, and allows one to determine which indicators are needed for a comprehensive and non-redundant assessment. (For more discussions see Section 2 and Figure S3 in the supplemental information.)

3 Discussion

3.1 Discussion of the results from the example

20   #### 3.1.1 What could we learn from the example?

As illustrated above, the SCoMaE method statistically evaluates the correlations between model output variables and uses this information to cluster variables, while selecting a representative indicator for each cluster. The exemplary analyses of the individual scenarios illustrates the dependence of the indicator selection on the imposed forcing scenario. These results demonstrate that for our model it is insufficient to apply the historical indicator set to the future scenarios with either higher

25   CO_2 forcing such as in the RCP8.5 scenario, or more limited CO_2 forcing and reduced anthropogenic land use such as in the RCP4.5 scenario. Although our analysis is too limited to conclusively determine a best set of climate change indicators in a purely scientific bottom-up approach, our results do suggest that a comprehensive assessment of future climatic states needs a re-evaluation of the ad-hoc chosen indicators, due to changes in prevailing climate responses.

We demonstrate one possible approach for selecting a more comprehensive indicator set by constructing a common correlation

30   matrix to identify indicators that can be used for the assessment of all three scenarios. For the clusters of variables of the common indicator set, the correlations remain significant even under different atmospheric carbon or land use forcing.

However, one should always ask if the identified clusters and indicators are scientifically meaningful? For the common cor-

relation matrix (as well as the RCP8.5 scenario), the first indicator, 'atmospheric CO_2' (A_co2), groups together variables describing changes in carbon fluxes, temperatures, and moisture fluxes over the ocean. This is scientifically meaningful, since changes in carbon fluxes will affect the atmospheric carbon content and hence atmospheric temperatures, both over land and ocean. These temperature changes in turn have an effect on the moisture fluxes over the ocean, such as the evaporation over

5 ocean, which is physically driven by temperature changes. These categories are hence physically linked and it is to be expected that they are correlated irrespective of the chosen forcing scenario.

The second indicator, 'precipitation over land' (F_precipL), represents the variability of moisture fluxes on land and the associated cooling effect. The fact that these processes are clustered under a indicator that is distinct from global and oceanic moisture fluxes indicates different underlying processes for these moisture fluxes, namely the influence of biological transpira-

10 tion. This process is directly affected by the parameter perturbations concerning the sensitivity of transpiration to CO_2 (Mengis et al., 2015) and the CO_2 fertilization effect (Matthews, 2007). Given the regarded parameter sensitivities of the model, the distinction between terrestrial and marine moisture fluxes is scientifically meaningful.

Another identified cluster is 'net top of atmosphere radiation' (F_netrad) and 'ocean surface heat flux' (F_heat), which are directly linked in the model. Furthermore 'net surface downward shortwave radiation' (F_dnswr) and 'land surface albedo'

15 (A_albsurL) are clustered, since changes in vegetation on land induced by the parameter perturbations, influence both the surface albedo on land and the incoming shortwave radiation at the surface.

The 'air to sea carbon flux' (F_carba2o) and 'soil respiration' (L_soilresp) are clustered together for all three scenarios, but show a negative correlation in the historical scenario and positive correlations in the two RCP scenarios, indicating a dependency on the atmospheric carbon concentrations. The predominant parameterization for those correlations is one that affects the

20 CO_2 fertilization (Figure S10). Since this is not an intuitive connection, we will shortly discuss this correlation in more detail: The strength of the CO_2 fertilization determines the increase of plant net primary production (NPP) to increasing atmospheric CO_2 concentrations. For the historical scenario, in the case when the CO_2 fertilization parameterization is increased, soil respiration increases due to an increase in vegetation and hence the soil carbon pool. In the same case the air to sea carbon flux slightly decreases due to lower atmospheric carbon concentration in case of increasing vegetation NPP and consequently land

25 CO_2 uptake. Hence the negative correlation between the 'air to sea carbon flux' (F_carba2o) and 'soil respiration' (L_soilresp) for the CO_2 fertilization perturbation in the the historical scenario (Figure S10a).

In contrast, in the future scenarios both Earth system variables are higher with increased CO_2 fertilization parameterization. For 'soil respiration' (L_soilresp) the underlying process remains the same in this case. However, the terrestrial carbon reservoir reaches a saturation state during the high emission scenarios. With increasing CO_2 fertilization strength the land carbon

30 reservoir reaches this saturation state earlier, causing more carbon to remain in the atmosphere, which results in an overall higher 'air to sea carbon flux' (F_carba2o) in the simulations with higher CO_2 fertilization, since the ocean equilibrates with the atmosphere. This explains the positive correlation under the two RCP scenarios.

Two clusters are identified in both future emission scenarios, namely 'ocean phytoplankton' (O_phyt), which is clustered with 'ocean surface phosphate' (O_po4sur) and 'ocean surface nitrate' (O_no3sur), and 'ocean oxygen' (O_o2), which is clus-

35 tered with 'ocean surface alkalinity' (O_alksur) (compare Figures S6 and S7). These two clusters are only identified when

atmospheric CO_2 concentrations are high, but do not hold for the historical scenario, where other relationships seem to be of greater importance. As a result, all of these variables are unclustered for the common indicator selection, causing the number of selected indicators for a common indicator set to increase.

3.1.2 Limitation of the analyses from the example

5 For our case study, we chose to assess the uncertainty of the biological system towards increasing temperature and CO_2, which is reflected in the choice of the considered perturbed parameters. In addition to directly perturbing biological parameterizations, we also perturbed some key physical parameters that indirectly influence the biological systems. All parameter perturbations were chosen because the parameterizations are poorly constrained and under future high CO_2 and temperature forcing it will be become increasingly important to take this uncertainty into account. These choices, however, bias the correlation analysis

10 of the model output variables towards their sensitivity to the selected perturbations (for a detailed discussion see Section 3 and Figure S4 in the supplemental information). For a more comprehensive assessment of uncertainties, experiments with different uncertainties in the simulated Earth system, such as cloud parameterizations or the model's climate sensitivity would need to be considered. Such experiments would accordingly change the patterns of the correlation matrix.

It is important to stress the fact that the Earth system variables used in our example are annual global integrals or means and

15 thus, not necessarily representative of regional or temporal changes. While our approach was sufficient to demonstrate the SCoMaE method, it is important to mention that global integrals and means are not always positively correlated to regional changes and therefore, may misrepresent regional responses. Furthermore, we restricted our case study to investigate temporal changes between two fixed points in time and thereby miss more detailed information about the temporal development of the response of the model variables to changes in parameter values. This approach was chosen since the UVic ESCM is a model

20 with low internal variability and would hence, likely overestimate information if we had evaluated temporal correlations. Investigating the model's sensitivity to the parameter perturbations was therefore deemed a better choice for illustrating the SCoMaE method. Any more thorough climate change assessment using the SCoMaE method would also need to investigate how variable correlations and indicator clusters might change spatially and temporally.

3.2 Discussion of the SCoMaE method

25 The construction of an individual or a common correlation matrix can be a useful tool for assessing the state of complex systems. Individual correlation matrices allow one to obtain an initial overview of relationships between the different system variables, whereas a common correlation matrix shows how changes in the state of a system, imposed by e.g. varying forcing scenarios, influences these relationships. The SCoMaE method then allows us to cluster the variables, based on statistical considerations, to obtain a non-redundant indicator set to guide more detailed analysis.

30 However, in order to be useful one must carefully select which information to include in the correlation matrix, which is something that strongly depends on the given research question. This can be illustrated by the implicit choices made for our exemplary case study, where we regarded correlations of globally averaged model output variables given various parameter perturbations. The first choice in this case study was to use global aggregates of the model output. However, if the research fo-

cus would be set on, e.g., regional phenomena the correlations for the matrix could also be constructed either between regional aggregates, or based on the correlation strength for a given spatial pattern.

The second choice we made for the case study was to regard correlations between model output variables based on their reaction to a parameter perturbation. Using a model with higher internal variability, it would also be possible to regard temporal correlations of a chosen time period, or other derivatives of the model output variables such as heat stress or cumulative time series. This would, in contrast to the purely process-based parameter perturbations, hold information about the time scales of the model output variables, which again might hints at common underlying processes in the model. Additionally, if the considered time series show higher internal variability it might be conceivable to apply a specific temporal filter to the data before calculating the correlation matrix. This might allow one to distinguish important processes on different time scales from daily and seasonal to inter-annual or decadal.

In the following we want to discuss the contribution of the SCoMaE method to achieve the three characteristics for indicator selection as introduced by Radermacher (2005). Constructing a correlation matrix enables scientists to comprehensively identify correlations in complex systems, such as the Earth system, both simulated and real. The application of SCoMaE allows one to identify scientifically consistent sets of indicators, which are independent and do not provide redundant information, to be used in a natural science-based assessments. This method represents a bottom-up, natural science perspective on indicator selection. It thereby tackles one of the three characteristics as discussed by Radermacher (2005), namely that of scientific consistency.

In our example the SCoMaE method is based on model data, and hence does not account for information about the statistical measurability of the identified indicators. This makes it difficult to directly translate a model-based indicator set to a 'real world' application. This is for example the case for the first indicator in the historical scenario, 'precipitation over ocean' (F_precipO), the lack of long term historical precipitation measurements over the ocean (New et al., 2001) would prevent this indicator from being used in a 'real world' application. It is however, noteworthy that there is value in the knowledge that this variable could hold information about other Earth system variables, and hence it might be worth improving the observational system.

The third characteristic mentioned by Radermacher (2005) is the political relevance of indicators. Since SCoMaE is a bottom-up, natural science-based approach for indicator selection, it at first disregards political, ethical and economical considerations. However, these considerations as well as measurability constraints can be included in the analysis. By prescribing a certain indicator, e.g. 'surface air temperature' (A_sat) in Section 2.5, SCoMaE allows us to include expert judgment and enables us to identify the remaining indicators needed for a fully comprehensive assessment. An iterative learning process of which indicators are needed and useful, would hence allow SCoMaE to identify a scientifically meaningful, measurable, and politically relevant indicators set (Oschlies et al., 2016; Singh et al., 2015).

4 Conclusions

In this study we introduced a bottom-up, correlation-based approach to systematically identify indicator sets for the assessment of complex systems. To demonstrate the power of the SCoMaE method, we applied it to correlation matrices constructed with Earth system variables of an intermediate complex Earth system model, with which we simulated three forcing scenarios. We were able to identify indicators sets for an assessment of the historical as well as for an intermediate high and a business as usual future emission scenario. The comparison of the three correlation matrices yielded the opportunity to assess changes in correlations between Earth system variables introduced by the imposed forcing. These changes in the correlation patterns also motivated a re-evaluation of the selected indicator sets for the different scenarios. We show that it is not sufficient to apply the indicator set identified for the historical scenario to the intermediate high nor the business as usual future emission scenario. This result points to the fact, that the classical procedure of ad-hoc indicators, such as surface air temperature, may work well for certain environmental conditions or scenarios, but possibly not so well for others. That is, the subjective choice of indicators may lead to unintended preferences in the interpretation of different scenarios. By combining the three scenarios into a common correlation matrix, we could identify correlations between Earth system variables that are robust across the three forcing scenarios. Considering these correlations only, enabled us to identify a common indicator set, which was scientifically consistent and allowed us to comparatively assess the three considered scenarios.

This case study is one example out of many possible applications of the correlation matrix and SCoMaE method. The construction of the correlation matrix can be adjusted to the respective research question, which makes the SCoMaE method a generic and flexible tool. An iterative application of the SCoMaE method offers the user the chance to comprehensively assess complex systems such as the Earth system, while including political, ethical and economical considerations, as well as measurability constrains.

Data availability. The model data used to generate the figures will be made available at http://thredds.geomar.de.

Appendix A: Model description

This paper illustrates the SCoMaE method for the example of model simulations performed with version 2.9 of the University of Victoria Earth System Climate Model (UVic ESCM), an Earth system model of intermediate complexity (Eby et al., 2013). It includes schemes for ocean physics based on the Modular Ocean Model Version 2 (MOM2) (Pacanowski, 1995), ocean biogeochemistry (Keller et al., 2012), and a terrestrial component including soil and vegetation dynamics (Meissner et al., 2003). It is coupled to a thermodynamic sea-ice model (Bitz et al., 2001) with elastic visco-plastic rheology (Hunke and Dukowicz, 1997). The atmosphere is represented by a two dimensional atmospheric energy moisture balance model (Fanning and Weaver, 1996). All model components have a common horizontal resolution of 3.6 ° longitude and 1.8 ° latitude and the oceanic component has a vertical resolution of 19 levels, with vertical thickness varying between 50 m near the surface to 500 m in the deep ocean. Wind velocities used to calculate advection of atmospheric heat and moisture as well as the air-sea-ice

fluxes of surface momentum, heat and water fluxes, are prescribed as monthly climatological wind fields from NCAR/NCEP reanalysis data (Eby et al., 2013). Wind anomalies, which are determined from surface pressure anomalies with respect to pre-industrial surface air temperature, are added to the prescribed wind fields.

A list of the globally aggregated output variables is given in Table S1.

A1   Spin-up and Scenario Forcing

For the default model simulation, the UVic ESCM was spun up with pre-industrial (year 1765) seasonal forcing for over ten thousand years. All simulations were integrated from 850 until 2005 using historical fossil-fuel emissions and land-use changes, as well as radiative forcing from solar variability and volcanic activity following Eby et al. (2013). Following Keller et al. (2014), continental ice sheets were held constant to facilitate the experimental setting and analyses. Warming from black carbon, indirect ozone effects, and cooling from indirect sulphate aerosol effects were not included. From 2005 onward until 2100 the Representative Concentration Pathway (RCP) 4.5 and 8.5 scenarios from Meinshausen et al. (2011) were implemented as an intermediate and high CO_2 emissions driven scenario, respectively.

For the sensitivity analysis performed with the UVic ESCM different model input parameters and parameterizations were perturbed, and for some of them it was necessary to do a new model spin-up to again reach steady-state conditions, apart from that the forcing was the same for all simulations.

Appendix B: Parameter Perturbations

In the following sections the single parameter perturbation experiments, which are used in the example and shown in Figure 1 are explained in detail. We chose these parameters to explore the sensitivity of the UVic ESCM to uncertainties in terrestrial and marine biological productivity with respect to temperature and CO_2, since these processes will influence the future carbon cycle. In addition, we perturbed ocean vertical diffusivity, since this is a physical process influencing marine carbon uptake. All parameters were perturbed within physically meaningful ranges, which was evaluated based on their agreement with the time series of the historical global mean air temperature and ocean heat content anomalies (manuscript in preparation by D. P. Keller). See Table B1 for a quick overview of the simulations.

B1   Vertical Ocean Diffusivity

Small-scale physical mixing (vertical diffusivity or diapycnal mixing) in the ocean is parameterized in all global models because of their resolution. Thus, this important process, which plays a key role in determining ocean circulation and bio-geochemical cycles as well as ocean to atmosphere heat and carbon fluxes, is set by necessity as a single global, or several regional, values that falls within the range of observational estimates of vertical diffusivity. To test how this affects all model results we varied this parameterization by increasing and decreasing it by 50% (Kv low and Kv high), which is within the range of observational estimates Duteil and Oschlies (2011). For these sensitivity analysis the model was spun-up with the

Table B1. List of perturbed model input parameters

Abbreviation	short explanation of parameter perturbation
Kv low	lower bound of vertical ocean diffusivity
Kv high	higher bound of vertical ocean diffusivity
no marine T sens	no marine biological sensitivity to temperature
no terr. T sens	no terrestrial vegetation sensitivity to temperature
veg q10 low	lower bound of the vegetation Q10 sensitivity
veg q10 high	higher bound of the vegetation Q10 sensitivity
soil q10 low	lower bound of the soil Q10 sensitivity
soil q10 high	higher bound of the soil Q10 sensitivity
CO_2 fert. zero	no CO_2 fertilization effect
CO_2 fert. low	lower bound of CO_2 fertilization effect
CO_2 fert. high	higher bound of CO_2 fertilization effect
transp. CO_2 sens zero	no CO_2 sensitivity of transpiration
transp. CO_2 sens low	lower bound of CO_2 sensitivity of transpiration
transp. CO_2 sens high	higher bound of CO_2 sensitivity of transpiration
CN CO_2 sens	stoichiometric changes in response to changing ocean carbonate chemistry

corresponding setting for 10000 years, until a new equilibrium climate state was reached.

B2 Lower Bounds of Biological Temperature Sensitivity

Although biological processes are known to be sensitive to temperature, there is a significant amount of uncertainty in how
5   biology will respond to warming caused by climate change (Friedlingstein et al., 2006; Taucher and Oschlies, 2011). Further-
more, there are many different ways to model the effects of temperature on biology and it is unknown which is best for Earth
system model applications. To investigate the lower bounds of the sensitivity of biological processes to direct temperature
effects we conduct simulations where direct temperature effects on biology are not included. In order to ensure that global
biogeochemical fluxes are as close to present-day ones as possible, flux-weighted global averages for temperature-dependent
10   rates were set for all temperature-dependent functions (see Taucher and Oschlies (2011) for details). This approach was applied
separately to marine and terrestrial ecosystems:

a) No marine biological sensitivity to temperature: The results of this analysis can be used to estimate a lower boundary
for how marine plankton and how their effect on biogeochemical cycles will respond directly to global warming (no marine T
15   sens). For this sensitivity analysis the model was spun-up with the corresponding setting for 10000 years, until a new equilib-

rium climate state was reached.

b) No terrestrial vegetation sensitivity to temperature: The results of this analysis can be used to estimate a lower boundary for how terrestrial vegetation and its effect on the carbon cycle will respond directly to global warming (no terr. T sens). For

5   this sensitivity analysis the model was spun-up with the corresponding setting for 10000 years, until a new equilibrium climate state was reached.

B3   Vegetation and Soil Sensitivity to Temperature

To further investigate the sensitivity of terrestrial biology to temperature we varied the vegetation and soil Q10 values, which are observationally-derived coefficients that are used to model the biological system rate of change in response to a 10 °C

10   temperature increase. Low and high Q10 values of 1.5 and 3.0 (model default is 2.0), which are within the range of observational estimates (Lloyd and Taylor, 1994), were set to investigate how different terrestrial biological sensitivities to temperature affects the model results (veg q10 low/high and soil q10 low/high). For this sensitivity analysis the model was spun-up with the corresponding setting for 10000 years, until a new equilibrium climate state was reached.

B4 CO_2 Fertilization of Vegetation

15   Increasing atmospheric CO_2 is thought to stimulate terrestrial carbon uptake, through the process of CO_2 fertilization (Matthews, 2007; Keenan et al., 2013). This negative carbon cycle feedback results in reduced atmospheric CO_2 concentrations, and has likely accounted for a substantial portion of the historical terrestrial carbon sink (Friedlingstein et al., 2006). However, the future strength of CO_2 fertilization in response to continued carbon emissions is highly uncertain. In order to test the impact of this uncertainty for future climate change simulations, we followed the approach of Matthews (2007) by scaling the CO_2

20   sensitivity of the terrestrial photosynthesis model. We performed a simulation with no CO_2 fertilization effect (CO_2 fert. zero), as well as two simulations where we varied the strength of the CO_2 fertilization effect by increasing and decreasing it by 50% (CO_2 fert. high/low) relative to the default model. No additional model spin-up was needed, since the simulated CO_2 fertilization effect only happens when the atmospheric CO_2 concentration begins to increase, e.g., from the preindustrial period onward.

25   B5 CO_2 Sensitivity of Transpiration

Transpiration by plants is highly sensitive to increases in atmospheric CO_2, since plants tend to open their stomata less often in higher CO_2 environments, in order to reduce water loss to the atmosphere. The strength of this effect and its impacts on climate are highly uncertain and has been studied both observation and model based (Keenan et al., 2013; Van Der Sleen et al., 2014; Mengis et al., 2015). To test how strongly this affects simulations of future climate, the amount of transpiration for all

30   plant functional types was scaled after Mengis et al. (2015). In this approach the CO_2 fertilization effect is not changed. Three simulations were performed: For the first simulation, transpiration did not change relative to the preindustrial level (transp.

CO$_2$ sens zero). For the other two simulations, the scaled transpiration was increased and decreased by 50% of the amount that the model would simulate with the default setting (transp. CO$_2$ sens high/low) as CO$_2$ changes. No additional model spin-up was needed, since the effect of changing CO$_2$ on transpiration only becomes evident when the atmospheric CO$_2$ concentration begins to increase, e.g., from the preindustrial period onward.

5 **B6 Stoichiometric Changes in Response to Changing Ocean Carbonate Chemistry**

Mesocosm studies that artificially increase the amount of CO$_2$ in seawater (e.g., climate change experiments) have suggested that the C:N content of marine plankton may be sensitive to changes in carbonate chemistry. The mesocosm study of Riebesell et al. (2007) suggested that as CO$_2$ increases the C:N content of phytoplankton may increases, which is a change that would affect the amount of carbon exported to the deep ocean by biological processes and have an effect on other marine

10 biogeochemical cycles. To test how this affects all model results we implemented the mesocosm-derived relationship between the atmospheric CO$_2$ concentration and the C:N content of plankton as in Oschlies et al. (2008) (CN CO$_2$ sens). No additional model spin-up was needed, since the effect of changing CO$_2$ on plankton stoichiometry only becomes evident when the atmospheric CO$_2$ concentration begins to increase, e.g., from the preindustrial period onward.

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