We thank the two reviewers for their very helpful comments on the manuscript, which have greatly improved the paper. Here we provide a point-by-point response of our proposed changes to the manuscript. The line numbers **in blue** refer to the marked-up version of the manuscript at the end of this document, which indicates how these proposed changes would integrate into the text.

Reviewer: Chris Brierley

This paper presents a meaningful step forward and an important clarification to the methodology of (paleo)climate factorisations. As such I would be happy to see it published following some small revisions.

I found the introduction of the synergy term in the Lunt et al (2012) factorisation a little bewildering at first. The manuscript didn't seem to contain an explanation as to why there is no need for a synergy term in the two-dimensional case. Is it because the averaging process effectively removes one degree of freedom (dimension)?

There is not really a "reason" why the Lunt et al (2012) factorisation is complete in two dimensions (i.e. does not require a synergy term) but is not complete for three or more dimensions (i.e. does require a synergy term) – two dimensions is just a special case. Added: "*Note that the Lunt et al (2012) factorisation is complete for N=2 without such a synergy term, but this is a case specific to N=2 as a result of cancellation of terms in Equation 4.*" See lines 111-114.

The re-analysis of the Chandan & Peltier paper is really nice. You do a good job of describing the impact of the different factorisations on it. However I was surprised there was no mention as to whether this reanalysis alters the conclusions of that original paper. Perhaps you would like to comment on that.

We checked the global mean values from the Chandan and Peltier study for each factorisation method and they differ by less than 10%. Added: *"The first thing to note is that the three factorisations all have very similar results; visually it is difficult to tell them apart on a regional scale, and they result in global means for each factor that differ by less than 10%. This is because, in this example, the non-linearities (i.e. the interaction terms) are relatively small. As such, the main conclusions of the Chandan and Peltier (2018) study are robust to a change in factorisation methodology."* See lines 289-293.

I, like the authors, and am a climate modeller and so I'm not abreast of relevant advances in other fields. I could not help wondering if this problem had been found and addressed outside of our discipline. Would you be able to comment?

**We have not found any discussion of the "problem" addressed in this manuscript in any previous work. However, we have expanded the introduction somewhat to include some more background and references to previous work: "*Factorisation experiments are used in many disciplines, with early applications being in agricultural field experiments (Fisher,1926), and widespread application in industrial and engineering design (Box et al., 2005) and other fields such as medicine (e.g. Smucker et al., 2019). The experiments that underpin such analysis are called 'factorial experiments'. In some cases, in particular when there are a large number of variables, not all combinations of all variables are tested (usually due to practical or computational limitations), and some previous work has focused on optimising the experimental design of such 'fractional factorial' experiments (e.g. Domagni et al., 2021). Furthermore, each test often has an associated error or uncertainty, and may be carried out multiple times. Analysis of such experimental designs is typically carried out using analysis of variance (ANOVA), in which the total change is represented as a model consisting of a series of 'main effects', one for each factor, and 'interaction effects' between the factors Montgomery (2013)…. In common with previously proposed factorisation methods in this field (Stein and Alpert, 1993; Lunt et al., 2012), we limit our analysis to the case where there are two possible values for*

***each variable, and where all combinations of all variables have been simulated; such an experimental design is called a 2^k (or two-level) full factorial experiment (Montgomery, 2013). Also in common with these studies, we assume that there is zero (or negligible) uncertainty in each simulation, which is consistent with the deterministic nature of most climate models.*”** **See lines 16-33.**

This manuscript has nine authors. Yet according to the "author contributions" statement only five have contributed to the work. Can you clarify why the others deserve authorship rather than a just credit in the acknowledgements?

We clarified the Author Contributions, which now read *"DJL led the study and wrote the first draft of the paper. GAS made Figure 3 and DC made Figure 4. DJL devised the linear-sum factorisation, GAS devised the shared-interaction factorisation, and GML devised the scaled-total factorisation. JCR provided the derivation of Equation 8. HJD, US, PJV, and AMH developed the boundary conditions and early Pliocene modelling that underpin the Pliocene simulations discussed. All authors contributed to writing the final version of the paper."* **See lines 338-341.**

L87. It took me a while to grasp this bracketed comment, although it actually seems quite important. Perhaps you could expand on it a little.

We expanded this comment, which now reads: *"This is apparent by considering the T_{111} terms; the three lines in Equation 5 each include a term equal to ¼ T_{111}, which sum to ¾ T_{111}, whereas they are required to sum to T_{111} for a complete factorisation. As such, an additional synergy term, S, in the sense of Equation 3, would be required for the factorisation to be complete in N=3 dimensions."* **See lines 107-110.**

L118. This sentence jarred with the 3/4 aside earlier. Why is it not 3/6 by the same logic?

Considering the T_{111} terms in Equation 6, there are three lines, each of which includes a term equal to 2/6 T_{111}, which sum to T_{111}.

L158. The wrong form of citation command is used here.

Corrected.

L160. f3 should be f2

Corrected.

L255. Please move the reference to fig 4a slightly earlier in the sentence.

Done.

Fig. 4 Can you please label the columns with the factorisation types?

We will do this.

Interactive Comment: Paul Pukite:

One way around this is to explain multiple phenomena with the same set of factors. A common-mode factor may emerge, thus ruling out factors that may be used in a model but are non-contributing with the entirety of the data.

Yes, this is correct, it is possible that a factorisation may reveal that one of the factors is larger than the others, and/or that some are relatively small. In our Pliocene example from the Chandan and Peltier (2018) paper this is not the case, as ice, CO_2 and orography are all the same order of magnitude in the global mean. There may be some confusion here between "Factor analysis" (https://en.wikipedia.org/wiki/Factor_analysis) and "Factorisation".

Reviewer: Anonymous Reviewer 2:

This study is well written, and very interesting. It presents a new development to Lunt et al., (2012) investigation of the factorization method used in paleoclimate modeling. The goal is to achieve completeness, uniqueness and symmetry of the factorization, and eliminate the synergy term. Mathematically, it is a fine solution. But I do have a couple questions:

The completeness is achieved by averaging out different additive paths of applying climate forcings (eq. 6) or sharing the synergy term proportionally with the generated warming by the individual "forcing" factors (eq. 15). I actually quite like the synergy term, because the synergy term has the physical meaning of capturing the non-linear effects of changing vegetation, ice sheet, topo/geography and CO2.

We agree that the synergy/interaction terms can be interesting and useful in some cases. We state this in the manuscript: "*These interaction terms are important and interesting, but there are cases where it can be useful or essential to only include attributable terms in the factorisation.*". See lines 125-126.

Beyond what is shown in Fig. 2, additional axes are needed to capture these non-linear effects. In fact, the points seemingly overlapping at T111 could be a visual illusion, and separable with additional axes of non-linear interactions. Wouldn't it be better to leave the synergy terms alone?

In Figure 2, the lengths of the various lines do not represent the magnitude of the individual temperature changes. It would require a 4th dimension show the temperature variable (challenging on a 2-dimensional pdf!). Similarly, in Figure 1 the temperature itself can be considered as a surface in a third dimension sitting above the 2-dimensional plane of CO_2 and ice sheet. We clarified this in the caption of Figure 1. However, even if we could represent this fourth dimension, then it would still be the case that the three lines in the top-right corner of Figure 2 would converge on a single point, T_{111}, because T_{111} is single-valued. Taking two example "routes" from the bottom-left (T_{000}) to the top-right (T_{111}), the overall change is, for one route: $(T_{100}-T_{000})+(T_{101}-T_{100})+(T_{111}-T_{101})$. For another route, it is $(T_{010}-T_{000})+(T_{011}-T_{010})+(T_{111}-T_{011})$. For both of these, terms cancel and they reduce to $T_{111}-T_{000}$. This is a mathematical property, not one associated with the climate system or the presence or absence of physical nonlinearities.

Additionally, Fig. 4 is a natural result of absorbing residuals into the calculation with corrections. I am worried that the physical meaning of factorization is contaminated through this absorption instead of being enhanced.

If researchers are interested in the synergy terms, then they can use the Stein and Alpert (1993) factorisation, or they can use our factorisations and still calculate the synergy terms from the Stein and Alpert (1993) factorisation. Added*: "In some cases, the interaction terms may, of course, be of great interest, and in such cases a non-pure factorisation can be very informative."*. See lines 330-332.

Specifically, how to interpret the differences between the left, middle and right column in a physically meaningful way? (- due to the attributions of nonlinear effect to different forcings?)

The differences between the left, middle, and right columns are related to the size of the synergy terms. With larger synergy terms (strong interactions between different factors), then the three columns would be more different to each other. The fact that the three columns look very similar is because actually, in this case, the synergy terms are relatively small. Added: "*The first thing to note is that the three factorisations all have very similar results; visually it is difficult to tell them apart on a regional scale, and they result in global means for each factor that differ by less than 10%. This is because, in this example, the non-linearities (i.e. the interaction terms) are relatively small.*" See lines 289-292.

For LGM, whether the symmetry is a feature of climate response to CO2 forcing is questioned (e.g., Zhu et al., 2020, Clim. Past. https://doi.org/10.5194/cp-2020-86). This study shows that changes in CO2 and ice sheet have different forcing efficacies under the LGM and preindustrial climate conditions. Similarly, asymmetric vegetation, ice sheet, and CO2 forcings might be prevalent for past climates. Would it be more useful to use the proposed framework to understand the asymmetry of climate forcings and responses instead of trying to force symmetry, which might not be a real feature in climate system?

We agree that there may be (in fact, almost certainly is!) an asymmetry in forcing and/or response of the climate system when considering the transition from preindustrial to a warm climate (e.g. the Pliocene), compared to a transition from the preindustrial to a cold climate (e.g. the LGM). This is a physical property of the climate system, related to the nonlinearity and/or state dependence of forcings and feedbacks. However, the "symmetry" that we discuss and define in this paper is not a physical property, but a mathematical one. It is the symmetry between the transition from preindustrial to LGM versus LGM to preindustrial. This is a mathematical requirement (A-B = -(B-A) !) . Here we "force" this symmetry, which we believe is the correct thing to do from a mathematical viewpoint – it does not preclude analysis of the type of physical "asymmetry" that the author refers to (B-A $\neq$ -(A-C)). In fact, the reviewer is basically saying that (in our 2-dimensional) case, T_{10}-T_{00} $\neq$ T_{11}-T_{01} ; which is certainly true in general, and fully consistent with our factorisation methodologies.

Lastly, this framework is described in the context of LGM, showing the LGM results would be more consistent.

We agree that it makes sense to be consistent between the initial examples and the applications to the previous work. As such, we changed the LGM example to a Pliocene example, by changing the names and by changing "warmer" to "colder" and vice versa, etc. See e.g. line 40-45.

<u>Other Changes:</u>

We made a number of minor typographical and grammatical corrections.

We added a note that the Lunt et al factorisation is identical to the 'main effects' in used in ANOVA. See line 113.

We added the additional concept of "purity", so that we can differentiate between completeness with and without a synergy term. See e.g. lines 72-73.

We removed the use of the term "synergy" (apart from in introduction), ad replaced with either "interaction term" or "residual" as appropriate, for consistency with some previous work. See e.g. line 98.

We added some more info to some of the captions. See e.g. Figure 1,4.

Multi-variate factorisation of numerical simulations

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Abstract. Factorisation is widely used in the analysis of numerical simulations. It allows changes in properties of a system to be attributed to changes in multiple variables associated with that system. There are many possible factorisation methods; here we discuss three previously-proposed factorisations that have been applied in the field of climate modelling: the linear factorisation, the Stein and Alpert (1993) factorisation, and the Lunt et al. (2012) factorisation. We show that, when more than two variables are being considered, none of these three methods possess all ~~three~~ four properties of 'uniqueness', 'symmetry', ~~and~~ 'completeness', and 'purity'. Here, we extend each of these factorisations so that they do possess these properties for any number of variables, resulting in three factorisations – the 'linear-sum' factorisation, the 'shared-interaction' factorisation, and the 'scaled-total' factorisation. We show that the linear-sum factorisation and the shared-interaction factorisation reduce to be identical in the case of four or fewer variables, and we conjecture that this holds for any number of variables. We present the results of the factorisations in the context of studies that used the previously-proposed factorisations. This reveals that only the linear-sum/shared-interaction factorisation possesses a ~~fourth~~ fifth property – 'boundedness', and as such we recommend the use of this factorisation in applications for which these properties are desirable.

1 Introduction

Factorisation (also called 'factor separation') consists of attributing the total change of some property of a system to multiple components, each component being associated with a change to an internal variable of the system. Multiple tests can be carried out to inform this factorisation, with each test (or simulation in the case of numerical applications) consisting of different combinations of variables. Factorisation experiments are used in many disciplines, with early applications being in agricultural field experiments (Fisher, 1926), and widespread application in industrial and engineering design (Box et al., 2005) ~~.~~ and other fields such as medicine (e.g. Smucker et al., 2019). The experiments that underpin such analysis are called ‘factorial experiments’. In some cases, in particular when there are a large number of variables, not all combinations of all variables are tested (usually due to practical or computational limitations), and some previous work has focused on optimising the experimental design of such ‘fractional factorial’ experiments (e.g. Domagni et al., 2021). Furthermore, each test often has an associated error or uncertainty, and may be carried out multiple times. Analysis of such experimental designs is typically carried out using analysis of variance (ANOVA), in which the total change is represented as a model consisting of a series of ‘main effects’, one for each factor, and ‘interaction effects’ between the factors (Montgomery, 2013).

In this paper, we focus on factorisation of numerical model simulations of the climate system; in this case, the factorisation typically consists of attributing a fundamental property of the climate system to multiple internal model parameters and/or boundary conditions~~(Stein and Alpert, 1993; Lunt et al., 2012).~~ . In common with previously proposed factorisation methods in this field (Stein and Alpert, 1993; Lunt et al., 2012), we limit our analysis to the case where there are two possible values for each variable, and where all combinations of all variables have been simulated; such an experimental design is called a 2^k (or two-level) full factorial experiment (Montgomery, 2013). Also in common with these studies, we assume that there is zero (or negligible) uncertainty in each simulation, which is consistent with the deterministic nature of most climate models. Factorisation has been ~~used~~ applied extensively in the climate literature; some ~~key~~ examples include Claussen et al. (2001), Hogrefe et al. (2004), van den Heever et al. (2006), and Schmidt et al. (2010); see also the collected studies in Alpert and Sholokhman (2011) . The factorisation method proposed by Stein and Alpert (1993) has currently been cited more than ~~250~~ 280 times according to Web of Science.

2 Previous factorisation methods

In order to introduce and discuss previous factorisation methods, we use an example case study from the field of climate science. We turn to the ~~Last Glacial Maximum (LGM), 21~~Pliocene, ~3 million years ago (Haywood et al., 2016, 2020; Dowsett et al., 2016) , ~~000 years ago ,~~ the most recent time ~~that the Earth has experienced a large-scale ice age. The LGM was 4–6~~ of prolonged natural global warmth relative to pre-industrial (Burke et al., 2018). The Pliocene oceans were on average about 2.5–3.5 °C ~~colder~~ warmer than pre-industrial ~~(Annan and Hargreaves, 2013; Snyder, 2016)~~(McClymont et al., 2020); for this example, we would like to know how much of this ~~cooling~~ warmth was due to ~~a decrease~~ an increase in atmospheric CO_2 concentration and how much was due to the ~~presence~~ reduction in extent and volume of large ice sheets. In this case we would use a climate model to carry out simulations with ~~various~~ combinations of high and low CO_2 concentrations, and with ~~and without~~ two different configurations of ice sheets. In general there are interactions between the variables so that the contributions from them do not ~~add~~ sum linearly.

It is worth at this stage introducing some notation. Here, we restrict ourselves to the case where there are two possible values for each variable, denoted ‘0’ and ‘1’; having more than two values increases the computational cost of a factorisation, and can reduce the number of factors that can be assessed in a fixed computing budget. We name the fundamental property of the climate system that we are factorising as T. If there are N variables, then the results of all possible simulations can be uniquely

Figure 1. ~~3~~ Three different factorisation methods of temperature, T, for ~~2~~ two variables (CO_2 and ice sheets). (a) Linear factorisation, (b) Stein and Alpert (1993) factorisation, (c) Lunt et al. (2012) factorisation. The temperature, T can be considered as a surface in a third dimension sitting above the 2-dimensional plane of CO_2 and ice sheets. In Equations 1,3, and 4, $\Delta T_1 = \Delta T_{CO2}$ and $\Delta T_2 = \Delta T_{ice}$.

identified by T followed by N subscripts of either 0 or 1, with each subscript representing the value of a variable, with the variables in some predefined order. For our ~~LGM~~ Pliocene example with two variables ($N = 2$), we have CO_2 (variable 1) and ice (variable 2) contributing to a global mean temperature (T); in this case there are 4 possible model simulations: a control (pre-industrial) simulation with pre-industrial CO_2 and pre-industrial ice (T_{00}), a second simulation with ~~LGM~~ Pliocene CO_2 and pre-industrial ice (T_{10}), a third simulation with pre-industrial CO_2 and ~~LGM~~ Pliocene ice (T_{01}), and ~~an LGM simulation with LGM~~ a Pliocene simulation with Pliocene CO_2 and ~~LGM~~ Pliocene ice (T_{11}) (see Figure 1a).

2.1 The linear factorisation

The simplest factorisation that can be carried out is a linear one. For the ~~LGM~~ Pliocene example with 2 factors, 3 simulations are carried out in which variables are changed consecutively; for example, T_{00}, T_{10}, and T_{11}. The factorisation of the total change, ΔT, between contributions due to CO_2 (ΔT_1) and ice (ΔT_2) would then be:

$$\begin{aligned} \Delta T_1 &= T_{10} - T_{00} \\ \Delta T_2 &= T_{11} - T_{10}. \end{aligned} \quad (1)$$

This factorisation is illustrated graphically in Figure 1(a). However, an equally valid linear factorisation would be

$$\begin{aligned} \Delta T_1 &= T_{11} - T_{01} \\ \Delta T_2 &= T_{01} - T_{00}, \end{aligned} \quad (2)$$

and in a non-linear system this would in general give a different answer to Equation 1. In this sense, the linear factorisation method is not 'unique'. However, it is 'complete' in the sense that the individual factors sum to the total change, ΔT exactly, i.e. $\Delta T_1 + \Delta T_2 = T_{11} - T_{00}$. Considering the linear factorisation as a 'path' starting at T_{00} and ending at T_{11}, it is also 'symmetric', in that if we instead started from T_{11} we would retrieve the same numerical values for the two linear factorisations (differing just by a minus sign for the numerical value of each factor). It is also 'pure' in that it does not need additional interaction terms (see Section 2.2 and Section 2.3) in order to make it complete.

2.2 The Stein and Alpert (1993) factorisation

Stein and Alpert (1993) proposed an alternative factorisation method, illustrated in Figure 1(b). In this, for the ~~LGM~~ Pliocene case, all four possible simulations are carried out, and the factorisation performed relative to the ~~preindustrial~~ pre-industrial case (T_{00}) for all variables. The non-linear terms are then all grouped together in ~~a term which is named~~ an interaction term

Figure 2. Simulations and linear factorisations in an $N=3$ factorisation. Edges that represent changes in CO_2 are in red, changes in ice are in blue, and edges in vegetation are in green. The paths associated with all three possible linear factorisations are shown with dotted lines.

(sometimes called the 'synergy'), S:

$$\begin{aligned} \Delta T_1 &= T_{10} - T_{00} \\ \Delta T_2 &= T_{01} - T_{00} \\ S &= T_{11} - T_{10} - T_{01} + T_{00}. \end{aligned} \quad (3)$$

In contrast to the linear factorisation, the Stein and Alpert (1993) factorisation is unique. It is also complete because $\Delta T_1 + \Delta T_2 + S = T_{11} - T_{00}$ (in fact, S is defined such that the factoristion is complete). ~~However,~~ As a result of the interaction term, S, it is not 'pure'. In addition, it is not symmetric; if we instead performed the factorisation relative to T_{11}, we would in general obtain a different numerical value of the factorisation (i.e. $\Delta T_1 = T_{01} - T_{11}$).

2.3 The Lunt et al (2012) factorisation

Lunt et al. (2012) proposed another factorisation, in which the factorisation for a particular variable is defined as the mean of the difference between each pair of simulations that differ by just that variable. This is illustrated in Figure 1(c); the factorisation of ice is represented by the mean of the two blue lines and the factorisation of CO_2 is represented by the mean of the two red lines:

$$\begin{aligned} \Delta T_1 &= \frac{1}{2}\left\{(T_{10} - T_{00}) + (T_{11} - T_{01})\right\} \\ \Delta T_2 &= \frac{1}{2}\left\{(T_{01} - T_{00}) + (T_{11} - T_{10})\right\}. \end{aligned} \quad (4)$$

The $N=2$ factorisation in Equation 4 is unique, complete, ~~and symmetric~~symmetric, and pure. It is worth noting that Equation 4 can be interpreted in multiple ways – either (i) as described above, the factorisation averages all the possible pairs of simulations that differ solely by a change in that variable, i.e. for a particular variable it is the mean of either the horizontal or vertical edges of the square in Figure 1(c); or (ii) it is the average of the two possible linear factorisations in Equations 1 and 2; or (iii) it is the average of the two possible Stein and Alpert (1993) factorisations obtained by swapping the ~~LGM~~ Pliocene and pre-industrial (in which case the ~~synergy~~ interaction terms cancel); or (iv) it is the Stein and Alpert (1993) factorisation but with the ~~synergy~~ interaction term, S, shared equally between the two factors.

In extending to $N=4$ variables, Lunt et al. (2012) assumed that the first of these interpretations would still hold for any number of variables. However, consider the $N=3$ case illustrated in Figure 2, in which we have added vegetation as a third variable to contribute to ~~LGM cooling~~Pliocene warming. Averaging the edges (interpretation (i) above) would result in a factorisation:

$$
\begin{aligned}
\Delta T_1' &= \frac{1}{4}\{(T_{100}-T_{000})+(T_{110}-T_{010})+(T_{101}-T_{001})+(T_{111}-T_{011})\}\\
\Delta T_2' &= \frac{1}{4}\{(T_{010}-T_{000})+(T_{110}-T_{100})+(T_{011}-T_{001})+(T_{111}-T_{101})\}\\
\Delta T_3' &= \frac{1}{4}\{(T_{001}-T_{000})+(T_{101}-T_{100})+(T_{011}-T_{010})+(T_{111}-T_{110})\}
\end{aligned}
\qquad (5)
$$

Although this is unique~~and symmetric,~~, symmetric, and pure, it is not complete, because $\Delta T_1'+\Delta T_2'+\Delta T_3' \neq T_{111}-T_{000}$~~(this is immediately~~. This is apparent by considering the T_{111} ~~term, for which~~ terms; the three lines in Equation 5 each include a term equal to $\frac{1}{4}T_{111}$, which sum to $\frac{3}{4}T_{111}$, whereas they are required to sum to T_{111} for a complete factorisation~~)~~. As such, an additional ~~synergy term, S,~~ interaction term, in the sense of S in Equation 3, would be required for the factorisation to be complete in $N=3$ dimensions ~~.~~ (in which case it would no longer be pure). Note that the Lunt et al. (2012) factorisation is complete for $N=2$ without such an interaction term, but this is a case specific to $N=2$ as a result of cancellation of terms in Equation 4. Note also that the Lunt et al. (2012) factorisation is equivalent to the ‘main effects’ term in ANOVA.

2.4 Summary of previous factorisations

As shown above, neither the linear, or the Stein and Alpert (1993), or the Lunt et al. (2012) factorisation methods possess all ~~three~~ four properties of uniqueness, symmetry, purity, and completeness in $N>2$ dimensions. These properties are often desirable in a factorisation, because any factorisation that lacks one of these properties is less easy to interpret. For example, for the ~~LGM~~ Pliocene example above, uniqueness means that we can have a single answer to the question “why is the ~~LGM colder than the preindustrial~~Pliocene warmer than the pre-industrial”. Symmetry means that we obtain the same answer to the question “why is the ~~LGM colder than the preindustrial~~Pliocene warmer than the pre-industrial” as to the question “why is the pre-industrial ~~warmer than the LGM~~colder than the Pliocene”. Completeness means that the answer to the question “how much warmer is the Pliocene than the pre-industrial” is equal to the sum of the individual factors (plus an interaction term if one exists). “Purity” means that we can answer the question ~~“~~“why is the ~~LGM colder~~ Pliocene warmer than the pre-industrial~~”~~” by referring solely to contributions from our fundamental factors CO_2, ice, and vegetation, i.e. without including additional ~~synergistic~~ interaction terms that are not attributed to a single factor. These ~~synergistic~~ interaction terms are important and interesting, but there are cases where it can be useful or essential to only include attributable terms in the factorisation.

3 Extensions to the previous factorisations

Here we discuss possible extensions to the three previous factorisations discussed above, that are unique, symmetric, pure, and complete in N dimensions.

3.1 Extension to the linear factorisation: The linear-sum factorisation

The linear-sum factorisation arises from a generalisation to $N>2$ dimensions of the second interpretation of Equation 4; i.e. it arises from averaging all the possible linear factorisations. This will result in a complete and pure factorisation because each individual linear factorisation is itself complete and pure. For three dimensions, this is illustrated by the dotted lines in Figure 2.

Each possible linear factorisation can be represented as a non-returning 'path' from the vertex T_{000} to the opposite vertex T_{111}, traversing edges along the way (dotted lines in Figure 2). When considering the sum of all possible paths, some edges are traversed more than others. In general, those edges near the initial or final vertices are traversed more times than edges that are further away from these vertices. As such, when we average the possible linear factorisations, different edges (corresponding to different terms in the factorisation) will have different weightings. This is in contrast to Equation 5 where each term (i.e. edge of the cube) has the same weighting. For three dimensions, Figure 2 shows that the 6 edges adjacent to the initial and final vertex are traversed twice, whereas the 6 other edges are traversed only once. Therefore, the factorisation is :

$$
\begin{aligned}
\Delta T_1 &= \frac{1}{6}\{2(T_{100}-T_{000})+(T_{110}-T_{010})+(T_{101}-T_{001})+2(T_{111}-T_{011})\} \\
\Delta T_2 &= \frac{1}{6}\{2(T_{010}-T_{000})+(T_{110}-T_{100})+(T_{011}-T_{001})+2(T_{111}-T_{101})\} \\
\Delta T_3 &= \frac{1}{6}\{2(T_{001}-T_{000})+(T_{101}-T_{100})+(T_{011}-T_{010})+2(T_{111}-T_{110})\}. \qquad (6)
\end{aligned}
$$

This factorisation is complete ($\Delta T_1 + \Delta T_2 + \Delta T_3 = T_{111} - T_{000}$), unique, ~~and symmetric~~symmetric, and pure.

To generalise to N dimensions, consider an N-dimensional cube, which has a total of 2^N vertices and $N \times 2^{N-1}$ edges. There are 2^{N-1} edges in each dimension. There are $N!$ paths from the initial vertex of the cube to the final opposite vertex, each of which consists of a traverse along N edges. Therefore, in each dimension there are a total of $N!$ edges traversed for all paths combined.

As for the 3-dimensional case above, let us label each vertex, V, of this N-dimensional cube as $V_{a_1 \cdots a_N}$, where each a_i is either 0 or 1. A value $a_i = 0$ represents the first value for variable i, and $a_i = 1$ represents the second value for variable i. Each vertex is also associated with a system value, denoted $T_{a_1 \cdots a_N}$ (see Figure 2 for the case $N = 3$).

All factorisations consist of partitioning the total change, $\Delta T = T_{1\cdots1} - T_{0\cdots0}$ between N factors. Each factor is associated with a dimension, i, in the N-dimensional cube. The factorisation for dimension i is ΔT_i.

For the linear-sum factorisation, all paths that we consider start at the origin vertex, $0\cdots0$, and end at the opposite vertex $1\cdots1$, and are made up of a series of edges. For all edges on the N-dimensional cube, let us define X as the set of all possible starting vertices, for a given N. For example, for $N = 3$, $X = \{000, 001, 010, 011, 100, 101, 110\}$. Let us define X_i as the set of all possible starting vertices for an edge that is oriented in the ith dimension, i.e. all those vertices that have a 0 in the ith subscript. For example, for $N = 3$ and $i = 2$, $X_2 = \{000, 001, 100, 101\}$. Let us define Y_i as the set of all possible ending vertices for an edge that is oriented in the ith dimension, so that Y_i is related to X_i by changing the ith subscript of each element from 0 to 1. For example, for $N = 3$ and $i = 2$, $Y_2 = \{010, 011, 110, 111\}$. Order X_i and Y_i so that their elements correspond. Then we write X_i^j to indicate the jth element of X_i, and Y_i^j as indicating the jth element of Y_i. For example, for the X_2 defined above, $X_2^3 = 100$.

The Lunt et al. (2012) factorisation averages along each edge oriented in dimension i:

$$\Delta T_i' = \frac{1}{2^{N-1}} \sum_{j=1}^{2^{N-1}} \left(T_{Y_i^j} - T_{X_i^j} \right) \tag{7}$$

For the linear-sum factorisation, we instead carry out a weighted average, with the weight for each edge in dimension i given by how many times it is traversed in all $N!$ paths. Consider all the paths that traverse an edge which starts at a vertex defined by k subscripts of '1' and $N-k$ subscripts of '0'. There are $k!$ possible paths to the start of this edge, and $(N-k-1)!$ paths from the end of this edge to the final corner (defined by N subscripts of '1'). Therefore, there are $k! \times (N-k-1)!$ paths that use this edge. As such, we can write the linear-sum factorisation as:

$$\Delta T_i = \frac{1}{N!} \sum_{j=1}^{2^{N-1}} \left\{ k_i^j!\,(N-1-k_i^j)!\,(T_{Y_i^j} - T_{X_i^j}) \right\}, \tag{8}$$

where k_i^j is the number of subscripts of '1' in X_i^j.

For example, for $N=4$ and $i=1$, we have $N!=24$ edges traversed in this dimension, and $2^{N-1}=8$ edges. $X_1 = \{0000, 0001, 0010, 0100, 0011, 0101, 0110, 0111\}$, and $Y_1 = \{1000, 1001, 1010, 1100, 1011, 1101, 1110, 1111\}$. For those edges with a starting subscript with $k=0$ subscripts of '1' (i.e. 0000), the weighting $k!\,(N-1-k)! = 0!\,(4-1-0)! = 6$. For those edges with a starting subscript with $k=1$ subscripts of '1' (i.e. $0001, 0010, 0100$), the weighting $k!\,(N-1-k)! = 1!\,(4-1-1)! = 2$. For those edges with a starting subscript with $k=2$ subscripts of '1' (i.e. $0011, 0101, 0110$), the weighting $k!\,(N-1-k)! = 2!\,(4-1-2)! = 2$. For those edges with a starting subscript with $k=3$ subscripts of '1' (i.e. 0111), the weighting $k!\,(N-1-k)! = 3!\,(4-1-3)! = 6$. Therefore, for $N=4$ and $i=1$, we have:

$$\begin{aligned}\Delta T_1 \;=\; & \frac{1}{24}\{6(T_{1000}-T_{0000}) + 2(T_{1001}-T_{0001}) + 2(T_{1010}-T_{0010}) + 2(T_{1100}-T_{0100}) + \\ & 2(T_{1011}-T_{0011}) + 2(T_{1101}-T_{0101}) + 2(T_{1110}-T_{0110}) + 6(T_{1111}-T_{0111})\}.\end{aligned} \tag{9}$$

3.2 Extension to the Stein and Alpert (1993) factorisation: the shared-interactions factorisation

As stated in Section 2.3, the Lunt et al. (2012) factorisation for $N=2$ can be interpreted as being identical to the Stein and Alpert (1993) factorisation but with the ~~synergy~~ interaction term shared between the two factors (thereby removing the interaction term, resulting in a pure factorisation). Here we explore what happens when this interpretation is generalised to $N>2$ dimensions. For consistency, we use the same notation as ~~(Stein and Alpert, 1993)~~Stein and Alpert (1993). In their notation, $\hat{f}_1$ represents the difference between a simulation in which only factor i is modified with a simulation in which no factors are modified, and $\hat{f}_{ijk...}$ represents interaction terms between the different factors. For example, for our original $N=2$ example illustrated in Figure 1 and given in Equation 3, $\Delta T_1 \equiv \hat{f}_1$, ~~$\Delta T_2 \equiv \hat{f}_3$~~$\Delta T_2 \equiv \hat{f}_2$, and $S \equiv \hat{f}_{12}$.

For our ~~LGM~~ Pliocene example for $N=3$, $\hat{f}_{12}$ is the interaction ~~term (i.e. the synergy)~~ between factors 1 and 2 (CO_2 and ice), $\hat{f}_{13}$ is the interaction ~~term~~ between factors 1 and 3 (CO_2 and vegetation), $\hat{f}_{23}$ is the interaction ~~term~~ between factors 2 and

Figure 3. (a) Visual representation of the shared-interaction factorisation for $N = 3$, as given by Equation 10. The straight dotted lines represent the sharing of the interactions according to Equation 11. (b) Visual representation of the shared-interaction factorisation for $N = 4$. The straight dotted lines represent the sharing of the interactions according to Equation 13.

3 (ice and vegetation), and $\hat{f}_{123}$ is the interaction ~~term~~ between all three factors. In this case, Stein and Alpert (1993) give that

$$
\begin{aligned}
\Delta T &= \hat{f}_1 + \hat{f}_2 + \hat{f}_3 + \hat{f}_{12} + \hat{f}_{13} + \hat{f}_{23} + \hat{f}_{123} \\
\hat{f}_1 &= T_{100} - T_{000} \\
\hat{f}_2 &= T_{010} - T_{000} \\
\hat{f}_3 &= T_{001} - T_{000} \\
\hat{f}_{12} &= T_{110} - (T_{100} + T_{010}) + T_{000} \\
\hat{f}_{13} &= T_{101} - (T_{100} + T_{001}) + T_{000} \\
\hat{f}_{23} &= T_{011} - (T_{010} + T_{001}) + T_{000} \\
\hat{f}_{123} &= T_{111} - (T_{110} + T_{101} + T_{011}) + (T_{100} + T_{010} + T_{001}) - T_{000}. \qquad (10)
\end{aligned}
$$

As discussed in Section 2.2, this factorisation is not symmetric or unique (e.g. we could define $\hat{f}_1 = T_{011} - T_{111}$) ~~, and it is only~~ or pure, but it is complete if we include all the interaction terms, which are not attributed to any particular factor. By extending the interpretation of ~~shared synergy~~ the shared interaction term in 2 dimensions discussed in Section 2.3, we can choose to share the interaction terms equally between their contributing factors, an approach applied by Schmidt et al. (2010) (although they carried out a ~~partial~~ fractional factorisation in which not all combinations of all variables were included). This results in a factorisation that is complete and pure (because we are just re-partitioning the interaction terms). It turns out that it is also symmetric. For example for CO_2,

$$\Delta T_1 = \hat{f}_1 + \frac{1}{2}\hat{f}_{12} + \frac{1}{2}\hat{f}_{13} + \frac{1}{3}\hat{f}_{123}. \qquad (11)$$

This factorisation for $N = 3$ is represented visually in Figure 3(a). Equations 10 and 11 give that, for CO_2,

$$\Delta T_1 = \frac{1}{6}\left\{2(T_{100} - T_{000}) + (T_{110} - T_{010}) + (T_{101} - T_{001}) + 2(T_{111} - T_{011})\right\}. \qquad (12)$$

This is identical to the equivalent term in Equation 6, indicating that the shared-interaction and linear-sum interpretations are identical for $N = 3$, and that therefore for $N = 3$ the shared-interaction factorisation is unique, symmetric, pure, and complete.

Stein and Alpert (1993) give the generalisation of their factorisation to N factors (their Equations 11-16). For $N = 4$, the interaction terms are shared so that, for example for CO_2,

$$\Delta T_1 = \hat{f}_1 + \frac{1}{2}(\hat{f}_{12} + \hat{f}_{13} + \hat{f}_{14}) + \frac{1}{3}(\hat{f}_{123} + \hat{f}_{124} + \hat{f}_{134}) + \frac{1}{4}\hat{f}_{1234}. \qquad (13)$$

This factorisation for $N = 4$ is represented visually in Figure 3(b). Again, for $N = 4$ this is ~~the same as the~~ identical to the linear-sum interpretation (Equation 9). We conjecture that for any N these two interpretations will give identical results.

3.3 Extension to the Lunt et al (2012) factorisation: The scaled-total factorisation

In the scaled-total factorisation, the Lunt et al. (2012) factorisation is modified so that it is complete (and remains pure). This is achieved by taking the total residual term required for completeness(the 'synergy', S in the sense of (Stein and Alpert, 1993)), , and sharing this between the factors in proportion to the sign and magnitude of their Lunt et al. (2012) factorisation. For the $N = 3$ example of the LGMPliocene, we have that the synergy, Sresidual term, R, is defined such that

$$\Delta T_1' + \Delta T_2' + \Delta T_3' + SR = T_{111} - T_{000}, \tag{14}$$

where the $\Delta T_i'$ are defined in Equation 5. We then share the synergy this residual proportionally across the three factors, such that

$$\begin{aligned}
\Delta T_1 &= \Delta T_1' + \frac{S\Delta T_1'}{\Delta T_1' + \Delta T_2' + \Delta T_3'}\frac{R\Delta T_1'}{\Delta T_1' + \Delta T_2' + \Delta T_3'} \\
\Delta T_2 &= \Delta T_2' + \frac{S\Delta T_2'}{\Delta T_1' + \Delta T_2' + \Delta T_3'}\frac{R\Delta T_2'}{\Delta T_1' + \Delta T_2' + \Delta T_3'} \\
\Delta T_3 &= \Delta T_3' + \frac{S\Delta T_3'}{\Delta T_1' + \Delta T_2' + \Delta T_3'}\frac{R\Delta T_3'}{\Delta T_1' + \Delta T_2' + \Delta T_3'}
\end{aligned} \tag{15}$$

Equations 14 and 15 reduce to:

$$\begin{aligned}
\Delta T_1 &= \Delta T_1' \frac{T_{111} - T_{000}}{\Delta T_1' + \Delta T_2' + \Delta T_3'} \\
\Delta T_2 &= \Delta T_2' \frac{T_{111} - T_{000}}{\Delta T_1' + \Delta T_2' + \Delta T_3'} \\
\Delta T_3 &= \Delta T_3' \frac{T_{111} - T_{000}}{\Delta T_1' + \Delta T_2' + \Delta T_3'}.
\end{aligned} \tag{16}$$

This shows that this factorisation can also be interpreted as simply scaling the Lunt et al. (2012) factorisation so that the sum of the factors equals $T_{111} - T_{000}$. In N dimensions, this generalises to:

$$\Delta T_i = \Delta T_i' \frac{T_{1\cdots 1} - T_{0\cdots 0}}{\sum_{j=1}^{N} \Delta T_i'} \tag{17}$$

where $\Delta T_i'$ is defined in Equation 7.

For example, for $N = 4$ and $i = 1$ we have:

$$\begin{aligned}
\Delta T_1' &= \frac{1}{8}\{(T_{1000} - T_{0000}) + (T_{1001} - T_{0001}) + (T_{1010} - T_{0010}) + (T_{1100} - T_{0100}) + \\
&\quad (T_{1011} - T_{0011}) + (T_{1101} - T_{0101}) + (T_{1110} - T_{0110}) + (T_{1111} - T_{0111})\} \\
\Delta T_1 &= \Delta T_1' \frac{T_{1111} - T_{0000}}{\Delta T_1' + \Delta T_2' + \Delta T_3' + \Delta T_4'};
\end{aligned} \tag{18}$$

and similarly for $\Delta T_2'$, $\Delta T_3'$, and $\Delta T_4'$.

4 Implications for previous published work

Here we discuss three examples of papers in which the Lunt et al. (2012) factorisation has been used. For each, we show how using our factorisations would affect the results in that paper.

4.1 Implications for Lunt et al (2012)

Lunt et al. (2012) presented a factorisation of global mean temperature change in the Pliocene ~~(3 million years ago, the most recent time of prolonged natural global warmth relative to pre-industrial)~~ into four variables: CO_2, orography, ice, and vegetation. As described in Section 2.3, in extending to $N = 4$ variables, the Lunt et al. (2012) factorisation is unique~~and symmetric,~~ , symmetric, and pure, but not complete. Using their notation, their factorisation for the CO_2 variable is (equivalent to Equation 9 in their paper):

$$dT'_{CO_2} = \frac{1}{8}\Big\{(T_c - T) + (T_{oc} - T_o) + (T_{ic} - T_i) + (T_{vc} - T_v) + (T_{ocv} - T_{ov}) + (T_{oci} - T_{oi}) + (T_{civ} - T_{iv}) + (T_{ociv} - T_{oiv})\Big\}. \quad (19)$$

The equivalent linear-sum/shared-interaction factorisation is given by Equation 9, which in the notation of Lunt et al. (2012) is:

$$dT_{CO_2} = \frac{1}{24}\Big\{6(T_c - T) + 2(T_{oc} - T_o) + 2(T_{ic} - T_i) + 2(T_{vc} - T_v) + 2(T_{ocv} - T_{ov}) + 2(T_{oci} - T_{oi}) + 2(T_{civ} - T_{iv}) + 6(T_{ociv} - T_{oiv})\Big\}, \quad (20)$$

and similarly for the other three variables.

The equivalent scaled-total factorisation is given by Equation 18, which in the notation of Lunt et al. (2012) is:

$$dT_{CO_2} = dT'_{CO_2}\frac{T_{ociv} - T}{dT'_{CO_2} + dT'_{orog} + dT'_{ice} + dT'_{veg}} \quad (21)$$

where dT'_{CO_2} is given in Equation 19; and similarly for the other three variables.

In Lunt et al. (2012), although Equation 19 (Equation 9 in their paper) was presented, the four variables were actually factorised by two $N = 2$ factorisations for all the analysis in that paper (Equation 13 in their paper). Because for $N = 2$ dimensions the Lunt et al. (2012), linear-sum/shared-interaction, and scaled-total factorisations are identical, the actual results related to Pliocene temperature change presented in Lunt et al. (2012) would not be affected by using our proposed new factorisations.

4.2 Implications for Haywood et al (2016)

Haywood et al. (2016), in the context of the experimental design for model simulations of the Pliocene in the PlioMIP project, presented a 3-variable factorisation of Pliocene warming into components due to CO_2, topography, and ice, based on the Lunt et al. (2012) factorisation (presented in their Section 3.2).

Figure 4. Comparison of various factorisation methods. (a) The mid-Pliocene minus preindustrial pre-industrial anomaly modeled ($T_{111} - T_{000}$) modelled by Chandan and Peltier (2017). (b–m) The top three rows present factorisations of the total anomaly into contributions arising from changes to CO_2 (upper, (b,f,j)), orography (middle, (c,g,k)) and ice sheets (lower, (d,h,l)), while the bottom row shows the residual required for completeness (‘synergy’), $T_{111} - T_{000} - (\Delta T_{CO_2} + \Delta T_{orog} + \Delta T_{ice})$, (e,i,m). Note that the residual term, R, for panel (e) is given by Equation 14, and is equal to $T_{111} - T_{000} - (\Delta T'_{CO_2} + \Delta T'_{orog} + \Delta T'_{ice})$. The first column (b,c,d,e) shows results using the methodology of Lunt et al. (2012) and is identical to results reported in Figure 7 of Chandan and Peltier (2018). The second column (f,g,h,i) shows results from the linear-sum/shared-interaction factorisation (Eq. Equation 6) and the third column (j,k,l,m) shows results of the scaled-total factorisation (Eq. Equation 16). The pink circles in the factorized results shown in the rightmost third column highlight regions where the scaled-total factorisation has very large negative or positive compensating values for the three factors, due to the very small values of denominator term appearing in Eq. 16 at those locations.

An alternative, using the linear-sum/shared-interaction factorisation that is complete, is obtained from Equation 6, which in their notation is, for CO_2 (and analogously for the other two components):

$$dT_{CO_2} = \frac{1}{6}\left\{2(E^{400} - E^{280}) + (Eo^{400} - Eo^{280}) + (Ei^{400} - Ei^{280}) + 2(Eoi^{400} - Eoi^{280})\right\} \tag{22}$$

Another alternative, using the scaled-total factorisation that is complete, is obtained from Equation 16, which in their notation is, for CO_2 (and analogously for the other two components):

$$\begin{aligned} dT'_{CO_2} &= \frac{1}{4}\left\{(E^{400} - E^{280}) + (Eo^{400} - Eo^{280}) + (Ei^{400} - Ei^{280}) + (Eoi^{400} - Eoi^{280})\right\} \\ dT_{CO_2} &= dT'_{CO_2} \frac{Eoi^{400} - E^{280}}{dT'_{CO_2} + dT'_{orog} + dT'_{ice}}. \end{aligned} \tag{23}$$

4.3 Implications for Chandan and Peltier (2018)

Chandan and Peltier (2018) applied the $N = 3$ factorisation of Lunt et al. (2012) (Equation 5), as also given by Haywood et al. (2016) (first line of Equation 23), to their suite of Pliocene simulations. The factorisation was applied to each gridcell in the model, resulting in $192 \times 288 = 55,296$ factorisations over the globe. The two-dimensional mid-Pliocene minus preindustrial temperature anomalypre-industrial temperature anomaly, reproduced here in Figure 4(a), was factorised into contributions originating from a change in CO_2, orography and ice sheets, and is reproduced here in Figure 4(a). Figure 4(b–d) shows the results of the original factorisation and is identical to those presented in Figure 7 of Chandan and Peltier (2018). Figure 4(f–h) shows the factorisation of the same anomaly using the linear-sum/shared-interaction method (Equations 22) while Figure 4(j–m) shows the results of employing the scaled-total method (Equations 23). The first thing to note is that the three factorisations all have very similar results; visually it is difficult to tell them apart on a regional scale, and they result in global means for each factor that differ by less than 10%. This is because, in this example, the non-linearities (i.e. the interaction terms) are relatively small. As such, the main conclusions of the Chandan and Peltier (2018) study are robust to a change in factorisation methodology.

The bottom row in Figure 4 shows, for the case of each method, the residual difference between the sum of all the factors and the total change (i.e. the ~~synergy~~ interaction/synergy terms in the sense of Stein and Alpert (1993)). The Lunt et al. (2012) method yields spatially coherent structures in the residual whose magnitude can be comparable to those of the factorized components, whereas the residuals for the other two methods are zero by definition, because they are ~~complete~~ pure (in the Figures they are very close to zero – essentially numerical noise due to round-off error). The non-linearity (indicated by the magnitude of the ~~synergy~~ residual term associated with the Lunt et al. (2012) factorisation) is greatest in the North Atlantic (Figure 4d), and is likely associated with changes in the sea-ice margin that are non-linearly influenced by all three boundary conditions (CO_2, orography, and ice sheets).

Figure 4(j–l) reveals a problem with the scaled-total method. In these panels, the pink circles show regions where the scaled-total factorisation has very large negative or positive values for the three factors. At these locations the denominator in Eq. 16 is very small, resulting in very large magnitude positive or negative results for each factorised components, which sum to a much smaller number. This is clearly not a meaningful result (because the values in the same region in Figure 4(a) are not unusual), and although in this analysis these issues are found to occur only at isolated locations, in other cases there is potential for the problem to be more widespread. In response to this, we introduce an a fourth property of factorisations – 'boundedness'. A factorisation is bounded if the factorisation for a particular variable (e.g. ΔT_1) is bounded by the minimum and maximum of all the possible single-factor factorisations for that variable. For example, for four dimensions, a factorisation is bounded if ΔT_1 has a value that is not greater than the largest, or smaller than the smallest, ~~term in~~ terms in the first line of Equation 18. The linear-sum/shared-interaction factorisation is by definition bounded, because it consists of a weighted average of those very terms. In contrast, the scaled-total factorisation is not bounded, and as such it should only be used with caution. It is worth noting that if absolute weightings were used in Equation 15, such that the scaled-total factorisation became (e.g. for CO_2):

$$\Delta T_1 \quad = \quad \Delta T_1' + \underline{\frac{S|\Delta T_1'|}{|\Delta T_1'|+|\Delta T_2'|+|\Delta T_3'|}}\,\frac{R|\Delta T_1'|}{|\Delta T_1'|+|\Delta T_2'|+|\Delta T_3'|}, \tag{24}$$

then the factorisation would not result in spuriously large values (because the denominator could never approach zero). However, the factorisation would still not be bounded in our definition. For example, if $\Delta T_1'$ were negative and consisted of all negative terms in the first line of Equation 5, ΔT_1 could still be positive if ~~S~~ R were sufficiently large.

5 Conclusions

In this paper, we have reviewed three previously-proposed factorisations, and extended them to produce factorisations that are unique, symmetric, pure, and complete. We have presented them for 3 dimensions (i.e. 3 factors), and generalised to N dimensions. The first factorisation, 'linear-sum' (Equation 8), averages all the possible linear factorisations on the N-dimensional cube. The second factorisation, 'shared-interaction', shares the interaction terms between each corresponding factor equally. The linear-sum and shared-interaction factorisations are shown to reduce to be identical for $N \leq 4$, and we conjecture that this holds for any N. The third factorisation, 'scaled-total' (Equation 17), averages all the contributions associated with the edges of the N-dimensional cube, and scales them by the total change in the property being factorised. We have presented re-

Table 1. Properties of the factorisations discussed in this paper.

[a] For these properties, we show that the properties hold for the linear-sum factorisation for N factors, and conjecture that the linear-sum and shared-interaction factorisations are identical.

sults of these extended factorisations in the context of previous work carried out by Lunt et al. (2012), Haywood et al. (2016), and Chandan and Peltier (2018) in the context of Pliocene climate change. This reveals that the scaled-total factorisation is not bounded, and therefore can lead to anomalous results that are hard to interpret. Therefore we recommend the use of the linear-sum/shared-interaction factorisation for cases where the properties of uniqueness, symmetry, ~~and~~ purity, completeness, and boundedness are desirable. In some cases, the interaction terms may, of course, be of great interest, and in such cases a non-pure factorisation can be very informative. Also, it is worth noting that if the interaction terms are zero, i.e. we have a completely linear system, then all the factorisation methods reduce to be identical. The properties of all the factorisations discussed in this paper are shown in Table 1 for 2,3,4, and N dimensions. The methods that we present here will be of particular use in the analysis of systems with multiple variables, and have application beyond solely climate science.

Code and data availability. The model fields underlying Figure 4 are available from the University of Toronto Dataverse in netcdf format: https://doi.org/10.5683/SP2/QGK5B0 . The python code used to calculate the factorisations illustrated in Figure 4 is available in the Supplement.

Author contributions. DJL led the study and wrote the first draft of the paper. GAS made Figure 3 and DC made Figure 4. DJL devised the linear-sum factorisation, GAS devised the shared-interaction factorisation, and GML devised the scaled-total factorisation. JCR provided the derivation of Equation 8. HJD, US, PJV, and AMH developed the boundary conditions and early Pliocene modelling that underpin the Pliocene simulations discussed. All authors contributed to writing the final version of the paper.

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