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Critical Analysis of the Path-Exchange Method for Hybrid Life-Cycle Assessment

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Abstract

Hybrid life-cycle assessment (HLCA) methods combine bottom-up data from process-based inventories with top-down data from environmentally extended input-output tables. This is done to overcome limitations of data coverage and aggregation: While process inventory data is more detailed, it can never be complete. On the other hand, input-output tables offer full cost-coverage for economic inventories that are complete, but highly aggregated into broad economic sectors. Combining these complementary datasets gives a more complete picture of the environmental impact associated with products or services. To this end, different mathematical methods have been proposed. Of the four main methods currently recognized in literature, three combine this data into a hybrid matrix. The path-exchange method instead works at the graph-level by combining the supply-chain paths of both systems. Unlike matrix-based hybrid methods, the accuracy of results of the graph-based method is limited by the number of paths considered. For the first time, we provide a concise mathematical description of the path-exchange algorithm and conduct a proof that this method is mathematically equivalent to the tiered-hybrid matrix method where upstream flows are inferred from the sectoral system. Based on this finding, we recommend the use of the method be discontinued in favor of the more accurate and computationally favorable matrix-based method, in combination with a structural path analysis of the resulting hybrid matrix. Our proof and the resulting guidance for practitioners is an important step toward a unified methodological framework for hybrid life-cycle assessment.

Keywords: hybrid life-cycle assessment, input-output life cycle assessment (IO-LCA), life cycle assessment (LCA), structural path analysis, environmental input-output analysis

1 Introduction

Since the early days of life-cycle assessment (LCA), researchers have attempted to combine data from complete but highly aggregated input-output tables of the economy with the incomplete but high-resolution process-based life-cycle inventory into a hybrid inventory. The first attempt was made in the 1970s [1], with most subsequent improvements made from the 1990s [2]. The umbrella term *hybrid life-cycle assessment* first saw use after 2000, for instance in a review by Lenzen et al. [3]. Today, it designates a number of distinct methods.

Four main methods have been recognized in literature [2][4]: The tiered method proposed in 1978 by Bullard et al. [1] and formalized by Heijungs et al. in 2002 [5], which was further formalized with respect to its harmonization of system boundaries to avoid double counting by Agez et al. between 2019 and 2022 [6]. The matrix augmentation method, introduced in 1999 by Joshi [7]. The integrated method, introduced in 2000 by Suh and Hupped [8]. Finally, the path-exchange (PXC) method, proposed in 1997 by Treloar [9] and formalized in 2009 by Lenzen et al. [10]. Despite recent publications aimed at establishing a standardized taxonomy [2], disagreement remains over the distinctions between methods.

Unlike the other three established methods, the path-exchange method operates at the level of the supply chain graph. This sets it apart from any matrix-based method. Its purported unique benefits, however, have remained somewhat elusive. For instance, the original authors have repeated statements of the kind *"Unlike other hybridisation methods, modifications to the supply chain are performed solely on discrete nodes, and thus do not require other changes within the overall matrix."* [11, Sec.2]. What this means for the utility of the method, for instance in the context of double-counting as described most recently by Agez et al. [6], has remained ambiguous. For instance, while some authors have described the path-exchange methods as employing *"algorithmic corrections for double-counting"* [12, Sec.6.1], others go further by claiming that it *"solves problems of double counting"* [4, Table 4] or that it *"cannot create any double-counting incident à la Strømman ([13])."* [14, Sec.2.6.3].

The original authors of the method in 2017 still observed that *"its application has been limited to a small group of scientists."* [11] and in 2018 *"(...) its application is rare and often limited to the group of researchers behind its development."* [2, Sec.5.2]. A systematic literature review shows that the path-exchange method for hybrid life-cycle assessment today is finding use primarily in the environmental assessment of the built environment, as shown in Table 2 of the Supplementary Information. Most recently, Stephan et al. were awarded the Graedel Best Paper Prize by the Journal of Industrial Ecology for their work on a *"multiscale framework for modeling and improving the life cycle environmental performance of built stocks"* [15], which employs this method.

Here, we describe the method in concise mathematical fashion, which allows us to illustrate the algorithm for a simple example system. Finally, we show that the method is, *in theory*, equivalent to the tiered hybrid matrix-based method for hybrid life-cycle assessment. We highlight the limitations inherent to any path-based algorithm, which mean that *in practice*, the path-exchange method will necessarily be inferior in accuracy to the matrix-based method. Based on this discussion, we caution practitioners against the use of this method. This comprehensive treatment will bring much-needed clarity to the ongoing discussion around the development of methods for hybrid life-cycle assessment.

2 Mathematical Framework

2.1 Example System and Diagrammatic Notation

We introduce an example system in Fig. 1, which we use extensively in Section 5. It consists of four economic sectors, and four production processes. We render the example system in a novel diagrammatic notation which allows for simple identification of process/sector correspondence, instances of double-counting, upstream flows from sectors to processes and the origin of data for every flow. This notation allows for an intuitive understanding of the hybridization of processes and sectors. It also allows us to augment the mathematical definition of the path-exchange method in Eq. (49) with a diagrammatic illustration in Fig. 3.

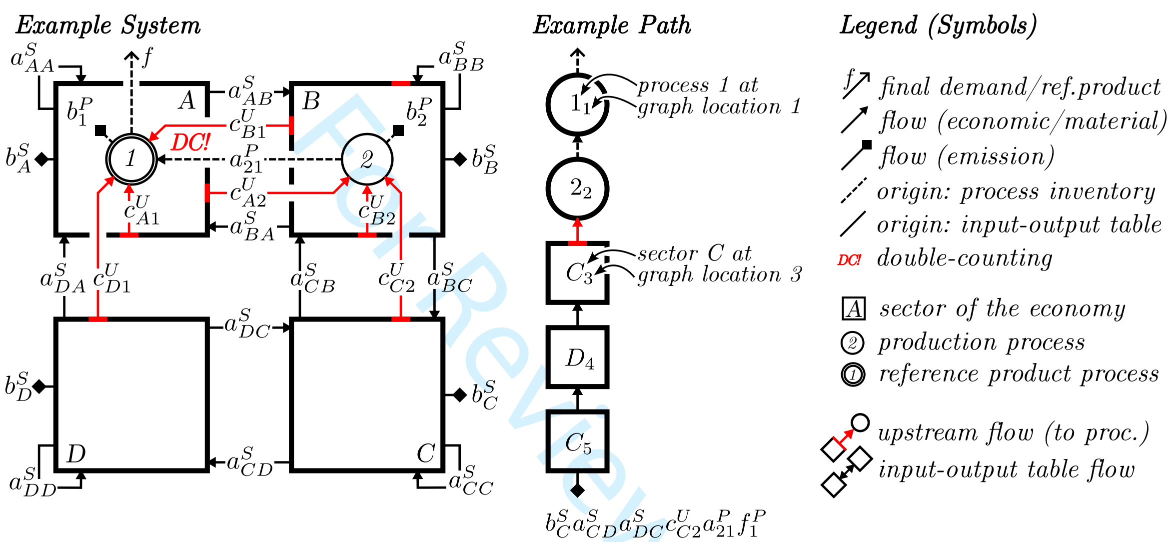

Figure 1: An example system of four sectors (A-D) and two processes (1,2), with corresponding matrices as defined in Eq. (1)-Eq. (3). Flows and emissions are annotated explicitly for the benefit of the reader. Note that not all sectors are connected to limit the complexity of the example. The diagrammatic notation is described in a legend presented in the right panel of the figure. This system is used in Fig. 3 and the mathematical proof of Section 4.

$$\mathbf{A}_S = \begin{array}{c} \\ A \\ B \\ C \\ D \end{array} \begin{array}{c} \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{bmatrix} a^S_{AA} & a^S_{AB} & 0 & 0 \\ a^S_{BA} & a^S_{BB} & a^S_{BC} & 0 \\ 0 & a^S_{CB} & a^S_{CC} & a^S_{CD} \\ a^S_{DA} & 0 & a^S_{DC} & a^S_{DD} \end{bmatrix} \end{array} \tag{1}$$

$$\mathbf{A}_P = \begin{array}{c} \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{cc} 1 & 2 \end{array} \\ \begin{bmatrix} 0 & 0 \\ a^P_{21} & 0 \end{bmatrix} \end{array} \tag{2}$$

$$\mathbf{H} = \begin{array}{c} \\ A \\ B \\ C \\ D \end{array} \begin{array}{c} \begin{array}{cc} 1 & 2 \end{array} \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \end{array} \tag{3}$$

2.2 Mathematical Convention and Table of Symbols

For the sake of simplicity in the equations of our proof but without loss of generality, we assume that both the process system and the sectoral system are already defined in the same units - either monetary or physical. For a detailed description of the conversion between these, we refer the reader to the comprehensive treatment by Weisz at al. [16].

For the sake of simplicity in our hybrid matrix representation, we have adopted the $\vec{e} = \mathbf{B}_P(\mathbf{I} - \mathbf{A_P})^{-1}\vec{f}_P$ convention for the governing equation of process-based life-cycle assessment. For a helpful discussion of the two different conventions, compare the comprehensive treatment by Heijungs et al. [17].

We employ the terms *node* and *edge* consistent with their standard usage in graph theory [18, P.9], where an *edge* is the flow between two *nodes*. In our case, a node could be a production process or economic sector, while an edge is the monetary of physical flow between them.

Table 1: Mathematical notation for vectors and matrices used throughout this article. The subscript P denotes the process system, the subscript S denotes the sectoral system and the subscript H denotes the hybrid system. For a complete derivation of the associated governing equations, refer to the supplementary information. Following formal notation in linear algebra [19, P.26], $\mathbf{A} \in \mathbb{R}^{R\times M}$ designates a matrix $\mathbf{A}$ of size $R \times M$ with all coefficients being elements of the real number field $\mathbb{R}$.

Index	*System*	*Description*
$i \in \mathbb{N}, \text{for } (1 \leq i \leq M)$	process system	production process ("activity")
$j \in \mathbb{N}, \text{for } (1 \leq j \leq N)$	sectoral system	economic sector
$k \in \mathbb{N}, \text{for } (1 \leq k \leq R)$	process system	environmental burdens (biosphere flows)
$l \in \mathbb{N}, \text{for } (1 \leq k \leq P)$	sectoral system	environmental burdens (env. satellite categories)

Matrix or Vector	*Description*
$\mathbf{A}_P \in \mathbb{R}_{M\times M}$	process system A-matrix (technology matrix [5])
$\mathbf{B}_P \in \mathbb{R}_{R\times M}$	process system environmental flow matrix (intervention matrix [5])
$\vec{f}_P \in \mathbb{R}_{M\times 1}$	final demand vector
$\vec{e}_P \in \mathbb{R}_{R\times 1}$	environmental flow vector
$\vec{x}_P \in \mathbb{R}_{M\times 1}$	output vector
$\mathbf{C}^u \in \mathbb{R}_{N\times M}$	upstream cut-off matrix
$\mathbf{A}_S \in \mathbb{R}_{N\times N}$	technical coefficient matrix
$\mathbf{B}_S \in \mathbb{R}_{P\times N}$	environmental satellite matrix
$\mathbf{H} \in \mathbb{R}_{N\times M}$	concordance matrix
$\vec{p} \in \mathbb{R}_{N\times 1}$	price vector

2.3 Matrix-Based HLCA Framework

Recent reviews recognize three distinct methods for hybrid life-cycle assessment which can be expressed in matrix form: the tiered hybrid method, the integrated hybrid method and the matrix-augmentation hybrid method [20][4][2]. While we must defer to these publications for detailed treatment of the different methods, we recapitulate the derivation of the tiered hybrid matrix method in the Supplementary Information for the benefit of the reader.

The basic assumption of the tiered hybrid method is that production processes consume inputs from other production processes. In addition, they consume "upstream" inputs from different sectors of the economy. Bearing in mind that a coefficient a_{ij} of the A-matrices defined in Table 1 describes the flow from node $i \rightarrow j$, we can consider a column of the A-matrix as the "production recipe" for the associated process or sector. With this, the governing equation of the tiered hybrid matrix method can therefore be written in the form most frequently used in literature:

$$\vec{e}_{H(tiered)} = \begin{pmatrix} \mathbf{B}_P & 0 \\ 0 & \mathbf{B}_S \end{pmatrix} \begin{pmatrix} \mathbf{I} - \mathbf{A}_P & 0 \\ \mathbf{C}_U^{uncorr} & \mathbf{I} - \mathbf{A}_S \end{pmatrix}^{-1} \begin{pmatrix} \vec{f}_P \\ 0 \end{pmatrix} \tag{4}$$

The uncorrected upstream cutoff matrix $\mathbf{C}_U$ contains all flows from sectors to processes. It can be populated *manually* by the practitioner. It can also be populated *automatically*, by inferring flows from the sectoral system, as first described by Strømman [21]. An intuitive illustration of this process is provided in Fig. 2. Here, process 1 originally only has inputs from process 2, which might reflect an incomplete system boundary, considering that its corresponding sector A requires inputs from both sector B and sector D. If the upstream cutoff matrix is automatically populated based on the requirements of sector A, it may compensate for missing flows from sector D. It also runs the risk, however, of doubly-counting some inputs. In this case from process 2 *and* sector B. This is instance of double counting illustrates the need for automated harmonization of the boundaries of the process and sectoral inventories through an automated correction for double counting.

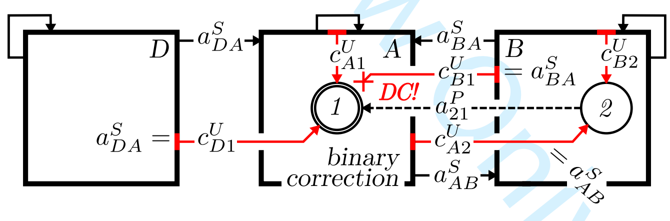

Figure 2: A simple example system consisting of three sectors (A,B,C) and two processes (1,2), taken the larger system in Fig. 1. Shown is the process by which upstream flows c^U are inferred from the sectoral system, as well as an instance of double-counting in a hybrid system ("DC!"). If both the upstream flow c^U_{C1} and the process flow a^P_{21} are retained, the environmental impact upstream of process 1 will be overestimated. Under the binary double-counting correction technique, the upstream flow c^U_{B1} is removed altogether. The upstream flow c^U_{D1} is not removed, since no process flow to process 1 originates in sector B. For a legend of the diagrammatic notation used, compare the right panel of Fig. 1.

The construction of the upstream matrix in this way can be formally defined as [21, Eqn.(4)ff.][6, Eqn.(7)]

$$\mathbf{C}_U^{uncorr} = \mathbf{A}_S \mathbf{H} \tag{5}$$

$$= \begin{array}{c} \\ A \\ B \\ D \end{array} \begin{array}{c} \begin{array}{ccc} A & B & D \end{array} \\ \begin{bmatrix} a^S_{AA} & a^S_{AB} & 0 \\ a^S_{BA} & a^S_{BB} & 0 \\ a^S_{DA} & 0 & a^S_{DD} \end{bmatrix} \end{array} \begin{array}{c} \\ A \\ B \\ D \end{array} \begin{array}{c} \begin{array}{cc} 1 & 2 \end{array} \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \end{array} \tag{6}$$

$$= \begin{array}{c} \\ A \\ B \\ D \end{array} \begin{array}{c} \begin{array}{cc} 1 & 2 \end{array} \\ \begin{bmatrix} c^U_{A1} = a^S_{AA} & c^U_{A2} = a^S_{AB} \\ c^U_{B1} = a^S_{BA} & c^U_{B2} = a^S_{BB} \\ c^U_{D1} = a^S_{DA} & 0 \end{bmatrix} \end{array} \tag{7}$$

Here, we first use the concordance matrix $\mathbf{H}$. As detailed in the Supplementary Information, a concordance matrix contains the information required to assign each process to one or more sectors of the economy. It can be used to convert vectors or matrices from the process-basis into the sector-basis. We define it as

$$\mathbf{H} \rightarrow h_{ij} = \begin{cases} 1 & \text{if sector } i \text{ contains process } j \\ 0 & \text{else} \end{cases} \tag{8}$$

As indicated in Fig. 2, this leads to potential cases of *double-counting*. These are instances in the hybrid system where an upstream flow from a sector into a process is already covered by a process flow. The upstream cut-off matrix must therefore be corrected to avoid double-counting. For a comprehensive discussion of different double-counting correction methods, compare the recent review by Agez et al. [6]. Here, we use the binary double-counting correction method[1]. Under this correction method, the upstream input from sector i into process j is set to zero, if any process flow to process j originates from a process contained in sector i. The concept is illustrated in Fig. 2. As we will see later, the path-exchange method essentially employs an identical logic.

In order to streamline the notation, we first introduce the Iverson bracket, which is a generalization of the Kronecker delta [23]. It is defined such that it evaluates to 1 if the condition in the bracket is true and evaluates to 0 otherwise. In our case, we use the condition

$$[x \overset{?}{=} 0] = \begin{cases} 1 & \text{if } x = 0 \\ 0 & \text{else} \end{cases} \tag{9}$$

where the question mark above the equality indicates that the expression is a logical condition evaluated by the Iverson bracket, rather than an assignment. Using the Iverson bracket notation and the definition of the concordance matrix, we can now formalize the equation which applies the binary double-counting correction technique to the uncorrected upstream flow matrix.

$$c_{ij}^{U,corr} = \left[\sum_{k=1}^{M} h_{ik} a^P_{kj} \overset{?}{=} 0 \right] c_{ij}^{U,uncorr} \tag{10}$$

According to the definition of the concordance matrix in Eq. (8)

$$h_{ik} a^P_{kj} = \begin{cases} a^P_{kj} & \text{if flow from process } k \rightarrow j \text{ originates in sector } i \\ 0 & \text{else} \end{cases} \tag{11}$$

and

$$M < i \leq N \ldots \text{index } i \text{ iterates over all } N \text{ sectors}$$
$$1 \leq j \leq M \ldots \text{index } j \text{ iterates over all } M \text{ processes}$$
$$1 \leq k \leq M \ldots \text{index } k \text{ iterates over all } M \text{ processes}$$

[1]Note that a small error is present in the equations for the corrected upstream cut-off matrix $\mathbf{C}_U^{corr}$ provided by Agez et al. [6, (8)-(8')]. Instead of the standard matrix multiplication the authors meant to use the Hadamard product [22].

We can see that the expression in the Iverson bracket evaluates to 1, only if no process in sector i has a flow a^P that terminates in process j. This is the definition of binary double-counting correction for hybrid life-cycle assessment. Using this notation, we can write corrected coefficients of the upstream flow matrix from the simple example in Fig. 2.

$$c_{B1}^{U,corr} = [0 \stackrel{?}{=} 0] c_{B1}^{U,uncorr} = c_{B1}^{U,uncorr} \tag{12}$$

$$c_{C1}^{U,corr} = [a_{21}^{P} \stackrel{?}{=} 0] c_{C1}^{U,uncorr} = 0 \tag{13}$$

In matrix form, Eq. (10) can be expressed as

$$\mathbf{C}_U^{corr} = [\mathbf{H}\mathbf{A}_P \stackrel{?}{=} 0] \otimes \mathbf{C}_U^{uncorr} \tag{14}$$

and the governing equation of the tiered hybrid matrix method becomes

$$\vec{e}_{H(tiered)} = \begin{pmatrix} \mathbf{B}_c^P & 0 \\ 0 & \mathbf{B}_c^S \end{pmatrix} \begin{pmatrix} \mathbf{I} - \mathbf{A}_P & 0 \\ \mathbf{C}_U^{corr} & \mathbf{I} - \mathbf{A}_S \end{pmatrix}^{-1} \begin{pmatrix} \vec{f}_P \\ 0 \end{pmatrix} \tag{15}$$

2.4 Path-Based HLCA Framework

As per the governing equation of both environmentally-extended input-output analysis and process-based life-cycle assessment, the environmental burden vector $\vec{e}$, which gives the total environmental burdens incurred from an arbitrary final demand $\vec{f}$, can be written as

$$\vec{e} = \mathbf{B}_c(\mathbf{I} - \mathbf{A})^{-1}\vec{f} = \mathbf{B}_c\mathbf{L}\vec{f} \tag{16}$$

In this context, $\mathbf{L}$ is known as the Leontief inverse. In the following, we will limit the discussion to the case of a single environmental burden (eg. carbon dioxide emissions). The above equation then becomes

$$e = \vec{b}_c^T\mathbf{L}\vec{f} \tag{17}$$

The first part of the equation is also known as the multiplier vector [24, Sec.6.2.3, Sec.8.5.1]

$$\vec{m}^T = \vec{b}_c^T\mathbf{L} \tag{18}$$

As originally proposed by Waugh [25] and reported by Miller & Blair from 1985 [26][27][24], the Leontief inverse $\mathbf{L} = (\mathbf{I} - \mathbf{A})^{-1}$ can be approximated by a power series, since $\sum_{i=1}^{n} a_{ij} < 1 \wedge a_{ij} \geq 0$ [24, Sec. 2.4.2].

$$\mathbf{L} = (\mathbf{I} - \mathbf{A})^{-1} = (\mathbf{I} + \mathbf{A} + \mathbf{A}^2 + \mathbf{A}^3 + \dots) \tag{19}$$

This is sometimes called *production layer decomposition* [10]. It forms the basis of both *structural path analysis*[2] in general and the path-exchange method for the *hybrid method* for life-cycle assessment in particular. A path in this context describes a product of coefficients of the kind $b_3a_{32}a_{21}$. These paths are formally known as directed acyclic graphs [18, P.200ff.]. With this, the environmental burden multiplier vector $\vec{m}^T$ in Eq. (18) can be expressed using the product layer decomposition in Eq. (19) as

$$m_i = b_i + \sum_{j=1}^{N} b_j a_{ji} + \sum_{j=1}^{N}\sum_{k=1}^{N} b_j a_{jk} a_{ki} + \sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N} b_j a_{jk} a_{kl} a_{li} + \dots \tag{20}$$

The path-exchange method now operates by combining paths from the production layer decomposition of a process system and a sectoral system. The associated algorithm is described in detail in Section 3.1. Similar to Eq. (15), we introduce the following notation to describe operation of the path-exchange method on both the sectoral and process paths

$$e = \mathrm{PXC}\{\mathbf{B}_c^S(\mathbf{I} - \mathbf{A_S}), \mathbf{B}_c^P(\mathbf{I} - \mathbf{A_P})^{-1}\}\vec{f}_P \tag{21}$$

[2] A detailed discussion of the evolving use of the term *structural path analysis* is provided in the Supplementary Information

3 The Path-Exchange Method for Hybrid Life-Cycle Assessment

3.1 General Description and Illustration

As detailed in Section 3.2, the path-exchange algorithm was first proposed by Lenzen et al. in 2009 [10]. Unfortunately, a formal mathematical or pseudo-code definition of this first implementation of the algorithm (hereafter named "PXC(2009)") was not provided. Instead, the different steps were traced out explicitly using a practical example.

Subsequent publications on the methodology of the path-exchange method by Crawford and Stephan et al. in 2017 [11] and 2019 [28] (hereafter named "PXC(2017/2019)") changed the definition of the method slightly [11, Sec.3.2][28, Sec.2.1]. No formal definition of the new implementation was provided either, although the method was visually illustrated in [11, Figure 2] and [28, Figure 1]. The method consists of multiple discrete steps, which we have illustrated in Fig. 3 using our novel diagrammatic notation.

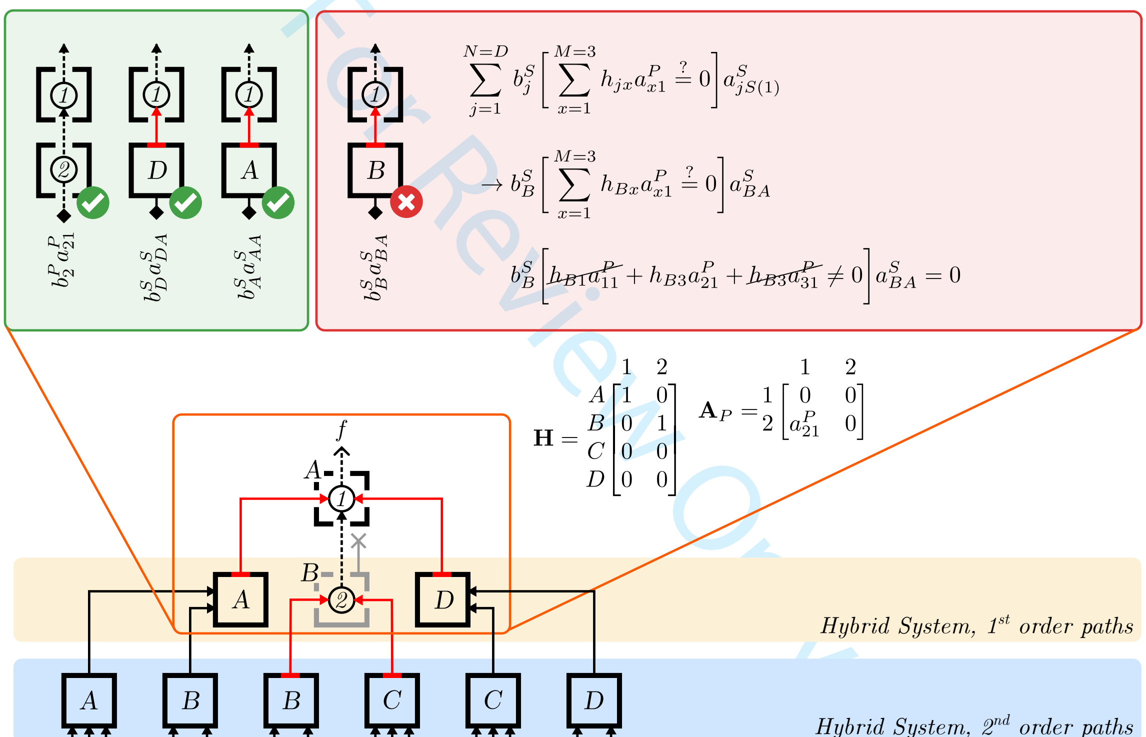

Figure 3: Visual representation of the PXC(2017/2019) algorithm, using the example system of Fig. 1. First, the algorithm conducts a structural path analysis of both the process system and the sectoral system. Of this, here we show only paths of orders 1-2 terminating in process 1. For order 1, we obtain one process path $b_2^P a_{21}^P$ and three sectoral paths $b_D^S a_{DA}^S, b_A^S a_{AA}^S, b_B^S a_{BA}^S$. Now, the algorithm *"matches"* the paths based on a concordance matrix **H**. In our diagrammatic notation, this is intuitively shown by process symbols being contained in sector symbols. Now, those sectoral paths are removed for which there is a direct process path equivalent. In this example, this is the case only for path $b_B^S a_{BA}^S$, which has the equivalent $b_2^P a_{21}^P$. Summing all paths according to Section 2.4 now yields the "hybrid" environmental impact. The mathematical formulation of this condition is shown next to the removed path. For a definition of the Iverson bracket operator used, compare Eq. (48). For a legend of the diagrammatic notation, compare the right panel of Fig. 1.

3.2 Historical Development and Motivation

Lenzen in his first complete formulation of the path-exchange method for hybrid life-cycle assessment describes his work [29, Sec.1] as building on the earlier method of Treloar [30, Sec.4], then referred to as *"an innovative input-output based hybrid analysis method"* [31, P.205]. He then asserts that *"The general decomposition approach* [used in the path-exchange method] *was introduced into economics and regional science in 1984 under the name Structural Path Analysis."*, citing Defourny et al. [32] and Crama et al. [33]. We find this representation of the lineage of the method to be incorrect, and present a more accurate version in Table 2. A detailed discussion of this lineage is presented in the Supplementary Information.

Table 2: Milestones in the historical development of the path-exchange method for HLCA.

authors	*year*	*contribution*	
Waugh	1950	power series expansion of the Leontief inverse	[25]
Bullard et al.	1975	power series expansion of the Leontief inverse and coefficient replacement	[34]
Seeman	1984	power series expansion of the Leontief inverse and coefficient replacement	[35]
Treloar	1997	refined method for coefficient replacement	[9]
Lenzen et al.	2009	first formalization in the context of life-cycle assessment	[36]
Crawford et al.	2017	workflow formalization	[11]
Stephan et al.	2019	software implementation	[28]

3.3 Motivation and Misconceptions

To support our formal proof in Section 4, we are providing a detailed discussion of three major misconceptions associated with the path-exchange method for hybrid life-cycle assessment in Section 3.3.1-Section 3.3.3. These misconceptions have all been used to motivate the introduction and use of the method and are among the reasons why the path-exchange method has so far been listed as a separate hybrid life-cycle assessment method in reviews publications.

3.3.1 "Avoiding Changing Coefficients in the Sectoral Matrix"

Treloar in his 1998 thesis motivated the introduction of his first version of the path-exchange method from two different perspectives: *"The process analysis framework cannot be used as a basis for hybrid analysis because of its incompleteness (ie, regardless of the greater reliability of the process analysis data). The comprehensive input-output framework cannot currently be used as basis for hybrid analysis because the substitution of process analysis data into the input-output model causes unwanted indirect effects."* [30, Sec.1].

The first point relates to the lack of available data for building the background inventory of a process-based life-cycle assessment. At that time, the *Ecoinvent* database predecessor *ETH 96* had just been released and featured less than 2'500 individual processes [37][38] - a number which has since increased to over 20'000 in the latest version [39][40]. The hope of Treloar was therefore to utilize readily available and up-to-date government-compiled input-output tables for better data coverage.

The interpretation of the second point is more involved and reveals an important misconception which has been frequently repeated since then. Treloar goes on to specify that *"(...) input-output-based hybrid analysis (...) involves the substitution of process analysis data for coefficients in the direct input-output matrix (Bullard et al., 1978 [1]; Seeman, 1984 [35])."* [30, Sec.2.3.2].

The concern here is that changes made to a technical coefficient of the input-output matrix in the context of one specific supply chain affect all other supply chains involving this technical coefficient.

This is an understandable concern in principle. However, the referenced publication by Bullard et al. does not modify the input-output matrix at all. It is instead an early example of input-output-based life-cycle assessment, as described most recently by Heijungs [17]. We must stress that the publication of Bullard et al. does not attempt to hybridize data, nor replace any coefficients in the input-output matrix, as claimed[3].

Similarly, the referenced thesis of Seeman does not modify the input-output matrix with more specific coefficients either. He briefly suggests a way to dis-aggregate sectors into more specific sub-sectors, thereby adding new columns and rows to the technical coefficient matrix. This approach would later be described in detail by Joshi [7] and is now commonly referred to as the *matrix-augmentation* hybrid method [2]. The calculations of Seeman, however, do not actually employ this dis-aggregation[4]. Instead, he describes a method for using the power series expansion of the Leontief inverse where input-output technical coefficients are replaced with more process-specific coefficients. This was already suggested by Bullard some 10 years earlier [34]. We must stress again that the publications of Seeman and Bullard et al. do not replace any coefficients in the input-output matrix, as claimed.

Apart from the integrated method for hybrid life-cycle assessment, where this is done deliberately, no hybrid analysis modifies the coefficients of the sectoral matrix. This includes the publications cited by Treloar. Note also that when Treloar made his proposal in 1997, the integrated method for hybrid life-cycle assessment had not yet been developed - and could therefore not have been referenced by him. Only two early publications by Bullard from 1976 [42] and 1978 [1] on what is today designated the tiered hybrid method had been published at the time.

Even so, this second point of the original motivation for the path-exchange method continued to be cited in subsequent publications: *"Treloar observed that changing the transaction coefficient for a particular element, or node, in an input-output matrix used for LCA would affect all supply chain paths that contain that node, even if the changed coefficients applied only to a particular path. Treloar correctly recognized that SPA provides a means to avoid such undesired "global" effects."* [10, Sec.1].

In summary, the second of two key issues cited as the original motivation for the introduction of the path-exchange method is not supported by the literature cited. It is plausible that it is based on a misinterpretation of the referenced publications.

[3] In the last paragraph, the theoretical possibility of "integrating" process data and input-output data is mentioned: *"With more extensive data, such as that from a conventional LCA, and a two-step process that integrates these data into the input-output matrix, we believe the two approaches can be integrated."* [41]. However, this *"integration"* is not described there in any further detail, nor is its implementation within the scope of the publication.

[4] The only change to the technical coefficient matrix that is made as part Seeman's calculations is the conversion of *"(...) the outputs of the energy sectors from dollars to megajoules (...)"* to facilitate the analysis of energy flows rather than economic flows.

3.3.2 "Working on Mutually Exclusive Nodes"

More recent publications on the path-exchange method have built on the misconception of Section 3.3.1 and listed as the main advantage of this approach that *"(...) it operates on mutually exclusive process and input output nodes"* [28, P.240] and that *"Unlike other hybridisation methods, modifications to the supply chain are performed solely on discrete nodes, and thus do not require other changes within the overall matrix."* [11, P.159].

This suggests that the path-exchange hybrid method, unlike matrix methods, can selectively modify nodes or edges in the supply chain pathways of a sectoral system and replace them with more precise nodes or edges from another system.

However, this is another misconception about the path-exchange method. In fact, selective replacement of sectoral information for process information at arbitrary locations in the supply chain graph can easily be achieved using a matrix-based system. As an example, consider a system illustrated in Fig. 4.

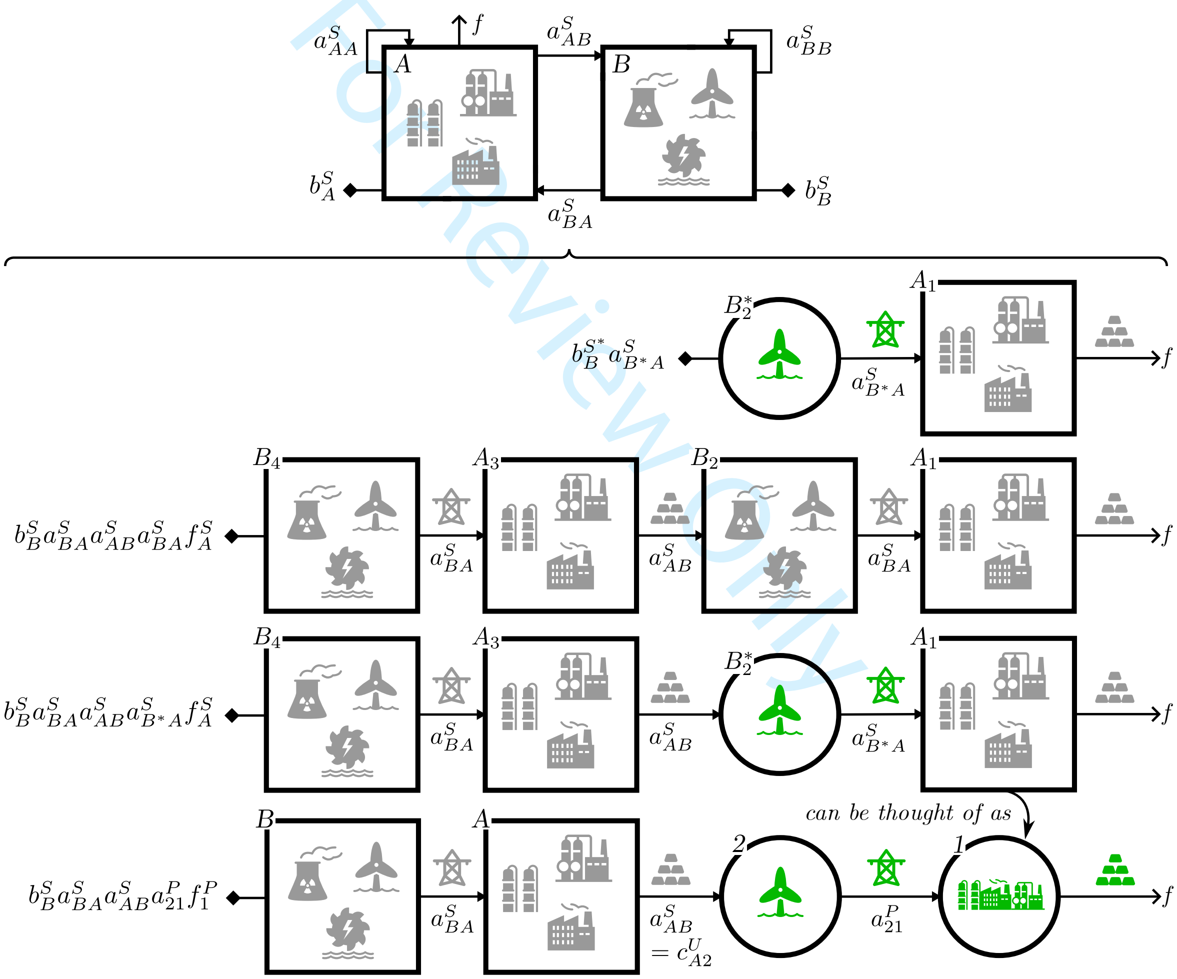

Figure 4: Top: A simple example system consisting of two sectors (A,B), taken the larger system in Fig. 1. Here, we assume sector A produces metals, while sector B supplies electricity. Bottom: An example path of order three: $b^S_B a^S_{BA} A^S_{AB} A^S_{BA} f^S_A$, in which a coefficient a^S_{BA} is exchanged for a more specific coefficient $a^S_{B^*A}$. For a legend of the diagrammatic notation, compare the right panel of Fig. 1.

We first posit that we have obtained specific information on edge $a^S_{B_2 A_1}$, the flow from the electricity sector into the metals sectors. In the following, we designate this specific node B^*. This includes data on the specific environmental burden of sector B $b^S_{B^*_2}$ and the amount of flow supplied to sector A $a^S_{B^*_2 A_1}$. Note that according to the legend in Fig. 1, the integer subscripts here indicate the position of the node or edge in the supply chain. The corresponding path

$$b^S_{B^*_2} a^S_{B^*_2 A_1} f^S_A \tag{22}$$

is shown in Fig. 4. Now, we consider an arbitrary third order path of the sectoral system. Note that the edge a^S_{BA} appears in different locations of this supply chain. It is underlined for emphasis.

$$b^S_{B_4} \underline{a^S_{B_4 A_3}} a^S_{A_3 B_2} \underline{a^S_{B_2 A_1}} f^S_A \tag{23}$$

According to Section 3.1, this path is now altered by the path-exchange method to

$$b^S_{B_4} a^S_{B_4 A_3} a^S_{A_3 B_2} a^S_{B^*_2 A_1} f^S_A \tag{24}$$

The path-exchange method has targeted a specific edge, denoted as $a^S_{B_2 A_1}$, at a particular point in the supply chain and replaced it with another edge instance, $a^S_{B^*_2 A_1}$, without altering other instances of the node-edge pair, such as $a^S_{B_4 A_3}$.

However, such a scenario can be easily captured in matrix form. The key to understanding this equivalence lies in the abstract notion that *specific information always lives on a specific supply chain.*

First, it is important to realize that in this example, we have information *only* on the electricity production node which feeds directly into the metal production node $B_2 \to A_1$. We have no information on electricity production nodes which appear *further upstream* in the supply chain, such as $B_4 \to A_3$.

To elaborate, consider again the first-order path of Eq. (22). In our scenario, we have specific information on the environmental burden coefficient $b^{S*}_{B_2}$ of node B at position 2 in the graph:

$$B_2 \to A_1 \to f \tag{25}$$
$$B^*_2 \to A_1 \to f \tag{26}$$

From Eq. (26) we can see that in our scenario we know *not only* something specific about node B_2, but *also* something about node A_1. At the very least, we know that in our specific supply chain, node A_1 does not consume the average input of node B_2, but the input of a specific node B^*_2. In our scenario, this is the only thing we know about node A_1. All other properties of this node we simply *infer* from the input-output system. These properties are the technical coefficient to this node a^S_{BA} and the environmental burden coefficient b^S_A.

We can therefore think of node A_1 as a *specific* node instance of sector A, much like B^*_2 is a *specific* node instance of sector B. For consistency, we therefore denote it A^*_1. This means that in our specific example, we have taken the metal production sector as a *proxy* for the metal production process under investigation.

How can we collect this specific information? One way to do so is in a process matrix $\mathbf{A}_P$ and an environmental burden coefficient vector $\vec{B}_P$. We can also think of these specific sectoral node instances (A_*, B_*) as processes $(1, 2)$.

$$\mathbf{A}_P = \begin{matrix} & A^* & B^* \\ A^* & 0 & 0 \\ B^* & a^S_{BA} & 0 \end{matrix} = \begin{matrix} & 1 & 2 \\ 1 & 0 & 0 \\ 2 & a^P_{21} = a^S_{BA} & 0 \end{matrix} \tag{27}$$

$$\vec{B}_P = \begin{matrix} A^* \\ B^* \end{matrix} \begin{bmatrix} b^S_A \\ b^{S*}_B \end{bmatrix} = \begin{matrix} 1 \\ 2 \end{matrix} \begin{bmatrix} b^P_1 = b^S_A \\ b^P_2 = b^{S*}_B \end{bmatrix} \tag{28}$$

We can see that in Eq. (27), the technical coefficient a^P_{21} between nodes B_2 and A_1 is simply the technical coefficient A^S_{BA}. Similarly, we can see that in Eq. (28), the environmental burden coefficient b^P_2 for node B_2 is simply the *specific* coefficient b^{S*}_B of which we have knowledge. The environmental burden coefficient b^P_1 for node A_1 is simply the sectoral average environmental burden coefficient b^S_A.

We know one more thing about node B_2. Since it is a specific instance of sector B, we can see from Fig. 4 that is takes input from sector A. We record this information in an upstream flow matrix $\mathbf{C}^U$.

$$\mathbf{C}^U = \begin{array}{c} \\ A \\ B \end{array} \begin{array}{c} \begin{array}{cc} 1 & 2 \end{array} \\ \begin{bmatrix} 0 & 0 \\ 0 & c^U_{A2} = a^S_{AB} \end{bmatrix} \end{array} \tag{29}$$

We can now, according to the definition of matrix-based methods for hybrid life-cycle assessment [2], combine this process matrix $\mathbf{A}_P$ with the input-output technical coefficient matrix $\mathbf{A}_S$. We do the same for the environmental burden coefficient vectors.

$$\mathbf{A}_H = \begin{array}{c|cc|cc} & 1 & 2 & A & B \\ \hline 1 & 0 & 0 & 0 & 0 \\ 2 & a^P_{21} = a^S_{BA} & 0 & 0 & 0 \\ \hline A & 0 & c^U_{A2} = a^S_{AB} & a^S_{AA} & a^S_{AB} \\ B & 0 & 0 & a^S_{BA} & a^S_{BB} \end{array} \tag{30}$$

$$\vec{B}_H = \begin{array}{c} 1 \\ 2 \\ A \\ B \end{array} \begin{bmatrix} b^P_1 = b^S_A \\ b^P_2 = b^{S*}_B \\ b^S_A \\ b^S_B \end{bmatrix} \tag{31}$$

Conducting a structural path analysis on the hybrid matrix in Eq. (30), we get:

$$m_1 \sim b^P_2 a^P_{21} + a^S_B a^S_{BA} c^U_{A2} a^P_{21} + \dots \tag{32}$$

This is equivalent to the path-exchange approach. As we can see, the matrix-based solution retains

$$B_4 \to A_3 \to B^*_3 \to A^*_1 \to f \tag{33}$$

In summary, it is key to understand that we *can* make modifications of specific nodes in a supply chain graph. However, this means that *all nodes downstream* of this modified node become specific node instances. We can infer their parameters from the input-output system and record them in a process matrix. This matrix can then be solved exactly according to the governing equation of input-output analysis $(\mathbf{I} - \mathbf{A})^{-1}\vec{f} = \vec{x}$ [24, Eqn.(2.11)].

3.3.3 "Avoiding Double Counting"

Another claim made by recent publications about the path-exchange method is that it *"avoids double-counting"* [10, Sec.4] as a result of *"exchange by definition"* [10, Sec.2.1]. This refers to the step of the path-exchange method that replaces some sectoral nodes with process nodes, leaving no *"ambivalence"* or double flows in these pathways.

However, this is another misconception about the path-exchange method. It does not somehow inherently avoid the problem of double counting. Instead, it simply employs the well-established binary double-counting correction method at the graph-level. As an example, consider a system illustrated in Fig. 5.

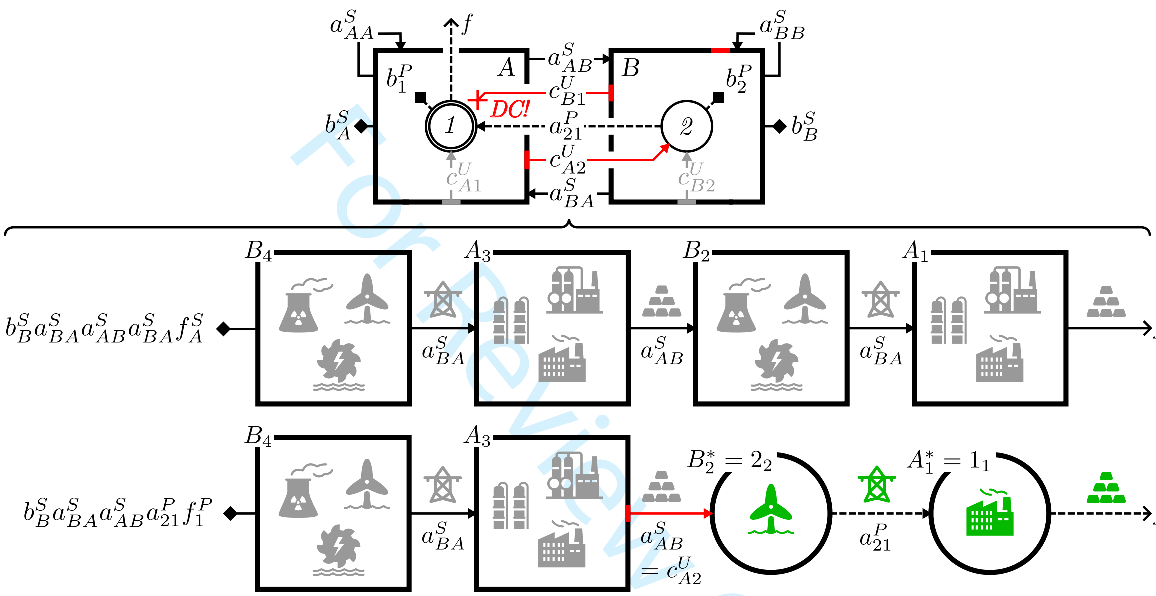

Figure 5: Top: A simple example system consisting of two sectors (A,B) and two processes (1,2), taken the larger system in Fig. 1. For the corresponding hybrid matrix, compare Eq. (37). Note that the two upstream flows c^U_{A1} and c^U_{B2} are not considered in the hybrid matrix for reasons of simlicity and are therefore shown in grey. As indicated by the line-style of the two red "upstream flow" arrows, they have been deduced from the underlying sectoral system. The resulting instance of double-counting is marked "DC!". As indicated by the terminating "X", flow c^U_{B1} is removed completely, therefore constituting binary double counting correction. For a legend of the diagrammatic notation, compare the right panel of Fig. 1. Bottom: Two example paths of the system: $b^P_2 a^P_{21} f^P_1$ and $b^S_B a^S_{BA} a^S_{AB} a^P_{21} f^P_1$.

Here, we again consider an arbitrary third order path of the sectoral system:

$$b^S_{B_4} a^S_{B_4 A_3} a^S_{A_3 B_2} a^S_{B_2 A_1} f^S_A \tag{34}$$

Note that according to the legend in Fig. 1, the integer subscripts here indicate the position of the node in the supply chain. As indicated in Fig. 5, specific information on two processes (1,2) is available. According to Section 3.1, the path is therefore altered by the path-exchange method to

$$b^S_{B_4} a^S_{B_4 A_3} a^S_{A_3 B_2} a^S_{2_2 1_1} f^P_1 = \tag{35}$$

$$b^S_{B_4} a^S_{B_4 A_3} c^S_{A_3 2_2} a^S_{2_2 1_1} f^P_1 \tag{36}$$

Note that here only the coefficient $a^S_{B_2 A_1}$ was changes, but not $a^S_{B_4 A_3}$.

The system of Fig. 5 can be represented through a hybrid technical coefficient matrix $\mathbf{A}_H$ and a hybrid environmental burden coefficient vector $\vec{B}$.

$$\mathbf{A}_H = \begin{array}{c} \\ 1 \\ 2 \\ A \\ B \end{array} \begin{array}{cccc} 1 & 2 & A & B \\ \hline 0 & 0 & 0 & 0 \\ a_{21}^P & 0 & 0 & 0 \\ 0(def!) & c_{A2}^U = a_{AB}^S & a_{AA}^S & a_{AB}^S \\ 0(DC!) & 0(def!) & a_{BA}^S & a_{BB}^S \end{array} \tag{37}$$

$$\vec{B}_H^T = \begin{array}{cccc} 1 & 2 & A & B \\ b_1^P & b_2^P & b_A^S & b_B^S \end{array} \tag{38}$$

As we can see from Eq. (37), the upstream flow c_{B1}^U into process 1 has been removed, because there is already a process flow a_{21}^P into process 1. This is the definition of binary double-counting correction. In the matrix this is indicated through "$0(DC!)$".

To *trace the supply chain paths* of this system, we now conduct a structural path analysis, following the description in Section 2.4. In the governing equation of environmentally extended input-output analysis, the environmental burden e associated with a final demand vector $\vec{f}_H$ can be expressed as

$$e = \vec{B}_H^T(\mathbf{I} - \mathbf{A}_H)^{-1}\vec{f}_H \tag{39}$$

The first part of this equation is known as the multiplier vector $\vec{m}$

$$\vec{m} = \vec{B}^T(\mathbf{I} - \mathbf{A})^{-1} \tag{40}$$

Using the power series expansion of a matrix inverse

$$(\mathbf{I} - \mathbf{A}_H)^{-1} = \mathbf{I} + \mathbf{A}_H + \mathbf{A}_H^2 + \ldots \tag{41}$$

we can expand the multiplier vector of Eq. (40). In our example, we consider the case where the functional unit is the output of process 1, as indicated in Fig. 5. The final demand vector is therefore simply

$$\vec{f}_H = \begin{array}{c} 1 \\ 2 \\ A \\ B \end{array} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{42}$$

According to Eq. (39) and Eq. (40), in this case the environmental burden e can be written as

$$e = \vec{m}\vec{f}_H \tag{43}$$

$$e = m_1 \tag{44}$$

and the power series expansion can be written as

$$m_1 = b_1^P + \sum_{j=1}^{4} b_j^H a_{j1}^H + \sum_{j=1}^{4}\sum_{k=1}^{4} b_k^H a_{kj}^H a_{j1}^H + \sum_{l=1}^{4}\sum_{j=1}^{4}\sum_{k=1}^{4} b_l^H a_{lk}^H a_{kj}^H a_{j1}^H + \ldots \tag{45}$$

We can now take a single third-order pathway from this expansion

$$b_4^H a_{43}^H a_{32}^H a_{21}^H = b_B^S a_{BA}^S c_{A2}^U a_{21}^P \tag{46}$$

This path is visualized in the bottom section of Fig. 5. As we can see, the binary double-counting correction in Eq. (37) ensures that no flow from sector B to process 1 is added. However, it does not impede the flow between sectors B and A elsewhere in the supply chain.

3.4 Limitations

In the structural path analysis of Eq. (20), the upper bound for the number of possible paths of order n for a system of N economic sectors is N^n. This holds true only if every node in the system is connected to every other node. Note that the exact number of possible paths in a more realistic system can only be computed by means of the adjacency matrix of the hybrid system, which we describe in the Supplementary Information. The equation for the upper bound of paths is frequently used incorrectly when referring to the number of possible paths [9, P.378][43, Footnote 1][36, P.8252][14, P.25]. Even limiting the investigation of paths to an arbitrary maximum path order may therefore prove computationally prohibitive, depending on the size of the system. To mitigate this issue, pruning techniques are used by practitioners, disregarding paths below a threshold contribution to overall impact [44, Sec.2.3]. These pruning techniques can be effective, reducing the number of relevant paths to a number much smaller than the total number of paths [45]. However, as practitioners note, a specific cut-of values is often chosen *"(...) for convenience, and because it was expected that it would provide a sufficiently detailed model to be used as the basis for an I–O-based hybrid analysis without providing too many energy paths."* [31]. And since most studies use systems of different size and scope, *"(...) subjective choices are unavoidable during the computational process."* [44].

One study combined the input-output table of the United Kingdom with the *Ecoinvent* database using the path-exchange method to investigate emissions of wind power. It was found that 23% of emissions were associated with paths that each contributed less than 0.034% [46, Supplement Sec.5]. As other authors observed, *"These small paths are often neglected in SPA studies ([47][29][48])."* [49]. One interesting example from a specific case study was provided: *"environmental impacts of electricity production in developing countries arise from numerous small contributions and not a few single, but large, contributions."* [49]. Any method working at the path-level is therefore subject to the above limitations. This is also the case for the path-exchange method for hybrid life-cycle assessment.

In addition, the error introduced by cutting of paths cannot be readily quantified. Error here refers to the missing amount of upstream input from the sectoral system into the process system, which is not accounted for due to the path cutoffs inherent to the path-exchange method. Since the number of possible paths grows exponentially with the size of the hybrid system, the traversal of these paths must be cut off after a specific threshold t of contribution to total emissions, or a specific path length d. In practice, authors have used varying parameters, depending on the study context $d = 5/t = 0.005 - 0.01\%$ [44], $d = 6/t = 5 - 1\%$ [48], $d = 8/t = 0.001\%$ [50], $d = 9/t = 0.001\%$ [49] or $d = 10/t = 0.1\%$ [51].

3.5 Mathematical Definition of the Path-Exchange Algorithm

Here, we provide the first ever formal mathematical description of the path-exchange algorithm. In Section 4, we will use this description to prove that the path-exchange method is equivalent to the tiered hybrid method. To show this, we will simply perform a structural path analysis on a matrix-based hybrid system and compare it to the formal description below.

As described in Section 3.1, a structural path analysis of the sectoral system and the process system is first performed. The key to a formal mathematical description of the algorithm is now the description of the logic it employs to add only some of the nodes of the sectoral system to the process system. The resulting paths then contain only the *"mutually exclusive nodes"* often cited as the distinction of the path-exchange method [11, Sec. 2][2, Sec.4][28, Sec.2.1].

As we can see in Fig. 3, only those paths from the sectoral SPA for which there is no corresponding process path are added. Consider, for instance, all first-order paths into sector $\boxed{A}$ in the example system of Fig. 1:

$$\sum_{j=1}^{N} b_j^S a_{jS(1)}^S = b_D^S a_{DA}^S + b_B^S a_{BA}^S \tag{47}$$

Here, the index subscript notation $S(1)$ refers to the sector which contains process 1. In the example system of Fig. 1, $S(1) \rightarrow A$ and therefore the sum $\sum_{j=1}^{N} a_{jS(1)}^S = a_{DA} + a_{BA}$.

First, we must determine whether there is any process with flows to process ① originating in sector $\boxed{B}$. As we can see from Fig. 1, process path a_{21}^P corresponds to sectoral path a_{BA}^S. Under the definition of the algorithm, this sectoral path must therefore not be added.

Again availing ourselves of the Iverson bracket notation Eq. (9) and the definition of the concordance matrix Eq. (8), we can write this condition as

$$\left[\sum_{i=1}^{M} h_{Bi} a_{i1}^P \stackrel{?}{=} 0\right] = \begin{cases} 1 & \text{if no process flow } a^P \text{ to process 1 originates in sector } B \\ 0 & \text{else} \end{cases} \tag{48}$$

The formal definition of the algorithm is now provided in Eq. (49). As we can see, the condition of Eq. (48) is used whenever sectoral paths are appended to a process path.

$$
\begin{aligned}
m_{1,pxc} = & \underbrace{\sum_{j=1}^{M} b_j^P \delta_{j1}}_{P:0^{\mathrm{th}}-\mathrm{order}} + \\
& + \underbrace{\sum_{j=1}^{M} b_j^P a_{j1}^P}_{P:1^{\mathrm{st}}-\mathrm{order}} + \underbrace{\sum_{j=1}^{N} b_j^S \left[\sum_{x=1}^{M} h_{jx} a_{x1}^P \stackrel{?}{=} 0 \right] a_{jS(1)}^S}_{S:1^{\mathrm{st}}-\mathrm{order}} + \\
& + \underbrace{\sum_{k=1}^{M} \sum_{j=1}^{M} b_k^P a_{kj}^P a_{j1}^P}_{P:2^{\mathrm{nd}}-\mathrm{order}} + \underbrace{\sum_{k=1}^{N} \sum_{j=1}^{M} b_k^S \left[\sum_{x=1}^{M} h_{kx} a_{xj}^P \stackrel{?}{=} 0 \right] a_{kS(j)}^S a_{j1}^P}_{S/P:2^{\mathrm{nd}}-\mathrm{order}} + \underbrace{\sum_{k=1}^{N} \sum_{j=1}^{N} b_k^S a_{kj}^S \left[\sum_{x=1}^{M} h_{jx} a_{x1}^P \stackrel{?}{=} 0 \right] a_{jS(1)}^S}_{S:2^{\mathrm{nd}}-\mathrm{order}} + \\
& + \underbrace{\sum_{l=1}^{M} \sum_{k=1}^{M} \sum_{j=1}^{M} b_l^P a_{lk}^P a_{kj}^P a_{j1}^P}_{P:3^{\mathrm{rd}}-\mathrm{order}} + \underbrace{\sum_{l=1}^{N} \sum_{k=1}^{N} \sum_{j=1}^{N} b_l^S a_{lk}^S a_{kj}^S \left[\sum_{x=1}^{M} h_{jx} a_{x1}^P \stackrel{?}{=} 0 \right] a_{jS(1)}^S}_{S:3^{\mathrm{rd}}-\mathrm{order}} + \\
& + \underbrace{\sum_{l=1}^{N} \sum_{k=1}^{N} \sum_{j=1}^{M} b_l^S a_{lk}^S \left[\sum_{x=1}^{M} h_{kx} a_{xj}^P \stackrel{?}{=} 0 \right] a_{kS(j)}^S a_{j1}^P + \sum_{l=1}^{N} \sum_{k=1}^{M} \sum_{j=1}^{M} b_l^S \left[\sum_{x=1}^{M} h_{lx} a_{xk}^P \stackrel{?}{=} 0 \right] a_{lS(k)}^S a_{kj}^P a_{j1}^P}_{S/P:3^{\mathrm{rd}}-\mathrm{order}} + \ldots
\end{aligned}
\tag{49}
$$

4 Proof of Mathematical Equivalency with Matrix Method

Despite previous reports in literature, the path-exchange method for hybrid life-cycle assessment does not constitute a distinct mathematical approach for integrating process and sectoral data. This has not been observed previously, as is evident by the treatment of this method in recent review publications [4][2]. In this section, we show the mathematical equivalence between the path-exchange method we formally defined in Section 2.4 and the matrix method we introduced in Section 2.3.

More specifically, we show the equivalence of the matrix method with binary double-counting correction where $\mathbf{C}^d = 0 \wedge \mathbf{C}^u \neq 0$.

Starting from the governing equation of the integrated hybrid matrix method in Eq. (15) and the governing equation of the path-exchange hybrid method in Eq. (21), we need to show that

$$\begin{aligned} \vec{e}_{H(pxc)} &= \mathrm{PXC}(\mathbf{B}_c^S(\mathbf{I} - \mathbf{A}^S)^{-1})\vec{f}^P = \\ &= \mathrm{PXC}(\mathbf{B}_c^S(\mathbf{I} + \mathbf{A}^S + (\mathbf{A}^S)^2 + (\mathbf{A}^S)^3 + \dots))\vec{f}^P \end{aligned} \tag{50}$$

$$= \vec{e}_{H(mx)} = \begin{pmatrix} \mathbf{B}^P & 0 \\ 0 & \mathbf{B}_c^S \end{pmatrix} \begin{pmatrix} \mathbf{A}^P & 0 \\ \mathbf{C}_{corr}^U & \mathbf{I} - \mathbf{A}^S \end{pmatrix}^{-1} \begin{pmatrix} \vec{f}^P \\ 0 \end{pmatrix} \tag{51}$$

In order to show the equivalence of Eq. (50) and Eq. (51), we must conduct a structural path analysis of the hybrid matrix in Eq. (51). The trick is to simply split up the row/column index into two indices, which go over $1 \leq i < M$ (processes) and $M \leq i \leq N$ (sectors). Note also that by the definition of the tiered hybrid matrix introduced in Section 2.3, the downstream flow matrix is zero and therefore all terms $\sum_{i=1}^{M} \sum_{j=M+1}^{N} a_{ij} = 0$. For convenience, the range of the row/column index combinations (i, j) is shown in Eq. (52):

$$\left[\begin{array}{c|c} 1 \leq i \leq M & 1 \leq i \leq M \\ 1 \leq j \leq M & M < j \leq N \\ \hline M < i \leq N & M < i \leq N \\ 1 \leq j \leq M & M < j \leq N \end{array}\right] \tag{52}$$

Note that in the upstream quarter of the matrix, where $M < i \leq N \wedge 1 \leq j \leq M$ the binary double-counting correction method from Eq. (10) must be applied. This means, that instead of the term

$$\sum_{i=M+1}^{N} \sum_{j=1}^{M} a_{ij}^H \tag{53}$$

in the decomposition, we get

$$\sum_{i=M+1}^{N} \sum_{j=1}^{M} \left[\sum_{k=1}^{M} h_{ik} a_{kj}^P \stackrel{?}{=} 0 \right] a_{ij}^H \tag{54}$$

Splitting up the indices, we can write:

$$
\begin{aligned}
m_{1,mx} = & \underbrace{\sum_{j=1}^{M} b_j^H \delta_{j1} + \cancel{\sum_{j=M+1}^{N} b_j^H \delta_{j1}}}_{H:0^{\text{th}}-\text{order}} \\
& + \underbrace{\sum_{j=1}^{M} b_j^H \boxed{a_{j1}^H} + \sum_{j=M+1}^{N} b_j^H \left[\sum_{x=1}^{M} h_{jx} a_{x1}^P \stackrel{?}{=} 0 \right] \boxed{a_{j1}^H}}_{H:1^{\text{st}}-\text{order}} \\
& + \underbrace{\sum_{k=1}^{M} \sum_{j=1}^{M} b_k^H \boxed{a_{kj}^H a_{j1}^H} + \sum_{k=M+1}^{N} \sum_{j=1}^{M} b_k^H \left[\sum_{x=1}^{M} h_{kx} a_{xj}^P \stackrel{?}{=} 0 \right] \boxed{a_{kj}^H} \boxed{a_{j1}^H} + \sum_{k=M+1}^{N} \sum_{j=M+1}^{N} b_k^H \boxed{a_{kj}^H} \left[\sum_{x=1}^{M} h_{jx} a_{x1}^P \stackrel{?}{=} 0 \right] \boxed{a_{j1}^H}}_{H:2^{\text{nd}}-\text{order}} \\
& + \underbrace{\sum_{l=1}^{M} \sum_{k=1}^{M} \sum_{j=1}^{M} b_l^H \boxed{a_{lk}^H a_{kj}^H a_{j1}^H} + \sum_{j=M+1}^{N} \sum_{k=M+1}^{N} \sum_{l=M+1}^{N} b_l^H \boxed{a_{lk}^H a_{kj}^H} \left[\sum_{x=1}^{M} h_{jx} a_{x1}^P \stackrel{?}{=} 0 \right] \boxed{a_{j1}^H}}_{H:3^{\text{rd}}-\text{order}} \\
& + \underbrace{\sum_{l=M+1}^{N} \sum_{k=M+1}^{N} \sum_{j=1}^{M} b_l^H \boxed{a_{lk}^H} \left[\sum_{x=1}^{M} h_{kx} a_{xj}^P \stackrel{?}{=} 0 \right] \boxed{a_{kj}^H} \boxed{a_{j1}^H} + \sum_{l=M+1}^{N} \sum_{k=1}^{M} \sum_{j=1}^{M} b_l^H \left[\sum_{x=1}^{M} h_{lx} a_{xk}^P \stackrel{?}{=} 0 \right] \boxed{a_{lk}^H} \boxed{a_{kj}^H a_{j1}^H}}_{H:3^{\text{rd}}-\text{order}} + \ldots
\end{aligned}
\tag{55}
$$

Comparing this to Eq. (49), we find all paths to be equal. □

This means that the power-series expansion of the system in Eq. (19) of a hybrid matrix like Eq. (15), which is constructed according the definition of the *tiered hybrid* method with binary double-counting correction, is equivalent to the paths returned by the *path-exchange hybrid* method.

5 Example

We illustrate the proof of mathematical equivalency from Section 4 by explicitly writing out all possible paths up to order 2 for the example system in Fig. 1. To simplify the equations, we assume the case of only a single environmental burden of interest (eg. carbon dioxide emissions). In addition, we place only a single unit of final demand on process 1, which is contained in sector A through a final demand vector

$$\vec{f}_P = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Using the definition of the path-exchange algorithm we introduced in Eq. (49) of Section 3.5, for paths up to order 2, the governing equation of the method can be written as

$$e_{1,H(pxc)} \sim \mathrm{PXC}\left\{ \sum_{j=1}^{N=4} b_j \left(\delta_{j1} + a^S_{j1} + \sum_{k=1}^{N=4} a^S_{jk} a^S_{k1} \right) \right\} \tag{56}$$

For illustrative purposes, we first separately write out the results of the structural path analyses of the process system and the sectoral system. The sub-paths of the sectoral system for which there is no correspondence with any sub-paths of the process system are underlined for better visibility.

$$\begin{aligned} \mathrm{SPA}(S) \sim & b^S_A + \\ & + \underline{b^S_A a^S_{AA}} + b^S_B a^S_{BA} + \underline{b^S_D a^S_{DA}} + \\ & + \underline{b^S_A a^S_{AA} a^S_{AA}} + \underline{b^S_A a^S_{AB}} a^S_{BA} + \underline{b^S_B a^S_{BA} a^S_{AA}} + \underline{b^S_B a^S_{BB}} a^S_{BA} + \underline{b^S_C a^S_{CB}} a^S_{BA} + \underline{b^S_C a^S_{CD} a^S_{DA}} + \underline{b^S_D a^S_{DD} a^S_{DA}} \end{aligned} \tag{57}$$

$$\begin{aligned} \mathrm{SPA}(P) \sim & b^P_1 + \\ & + b^P_2 a^P_{21} + \\ & + b^P_3 a^P_{32} a^P_{21} \end{aligned} \tag{58}$$

The path-exchange algorithm now goes to work and returns:

$$\begin{aligned} e_{1,H(pxc)} \sim & b^P_1 + \\ & + \underline{b^S_A a^S_{AA}} + b^P_2 a^P_{21} + \underline{b^S_D a^S_{DA}} \\ & + \underline{b^S_A a^S_{AA} a^S_{AA}} + \underline{b^S_A a^S_{AB}} a^P_{21} + \underline{b^S_B a^S_{BA} a^S_{AA}} + \underline{b^S_B a^S_{BB}} a^P_{21} + \underline{b^S_C a^P_{CB}} a^P_{21} + \underline{b^S_C a^S_{CD} a^S_{DA}} + \underline{b^S_D a^S_{DD} a^S_{DA}} \end{aligned} \tag{59}$$

Now, we construct the hybrid matrix of the example. This will allow us to perform a structural path analysis on the hybrid matrix and compare it to Eq. (59).

$$\mathbf{A}_H = \begin{array}{c} \\ 1 \\ 2 \\ A \\ B \\ C \\ D \end{array} \begin{array}{cc|cccc} 1 & 2 & A & B & C & D \\ 0 & 0 & 0 & 0 & 0 & 0 \\ a^P_{21} & 0 & 0 & 0 & 0 & 0 \\ \hline c^U_{A1} = a^S_{AA} & c^U_{A2} = a^S_{AB} & a^S_{AA} & a^S_{BA} & 0 & 0 \\ c^U_{B1} = 0 (DC!) & c^U_{B2} = a^S_{BB} & a^S_{BA} & a^S_{BB} & a^S_{BC} & 0 \\ 0 & c^U_{C2} = a^S_{CB} & 0 & a^S_{CB} & a^S_{CC} & a^S_{CD} \\ c^U_{D1} = a^S_{DA} & 0 & a^S_{DA} & 0 & a^S_{DC} & a^S_{DD} \end{array}$$

We can now perform the structural path analysis on this matrix:

$$e_{1,H(mx)} \sim \sum_{j=1}^{M+N=2+4} b_j^H \left(\delta_{j1} + a_{j1}^H + \sum_{k=1}^{M+N=2+4} a_{jk}^H a_{k1}^H \right) \tag{60}$$

$$\begin{aligned}
=& b_1^H + \\
&+ b_2^H a_{21}^H + b_3^H a_{31}^H + b_6^H a_{61}^H + \\
&+ b_3^H a_{32}^H a_{21}^H + b_4^H a_{42}^H a_{21}^H + b_5^H a_{52}^H a_{21}^H + b_4^H a_{43}^H a_{31}^H + b_3^H a_{33}^H a_{31}^H + b_5^H a_{56}^H a_{61}^H + b_6^H a_{66}^H a_{61}^H
\end{aligned} \tag{61}$$

$$\begin{aligned}
=& b_1^P + \\
&+ b_2^P a_{21}^P + b_A^S c_{A1}^U + b_D^S c_{D1}^U + \\
&+ b_A^S c_{A2}^U a_{21}^P + b_B^S c_{B2}^U a_{21}^P + b_C^S c_{C2}^U a_{21}^P + b_A^S a_{AA}^S c_{A1}^U + b_B^S a_{BA}^S c_{A1}^U + b_C^S a_{CD}^S c_{D1}^U + b_D^S a_{DD}^S c_{D1}^U
\end{aligned} \tag{62}$$

$$\begin{aligned}
=& b_1^P + \\
&+ b_2^P a_{21}^P + b_A^S a_{AA}^S + b_D^S a_{DA}^S \\
&+ b_A^S a_{AB}^S a_{21}^P + b_B^S a_{BB}^S a_{21}^P + b_C^S a_{CB}^P a_{21}^P + b_A^S a_{AA}^S a_{AA}^S + b_B^S a_{BA}^S a_{AA}^S + b_C^S a_{CD}^S a_{DA}^S + b_D^S a_{DD}^S a_{DA}^S
\end{aligned} \tag{63}$$

Comparing Eq. (59) and Eq. (63), we find them to be equal. Note that the paths listed in these equations can be also visually traced in the diagrammatic representation of the example system in Fig. 1.

6 Computational Intensity

Finally, we find that the path-exchange method for hybrid life-cycle assessment is significantly more computationally expensive than any matrix-based method. This is because covering a large enough number paths to obtain a high degree of emissions coverage in life-cycle assessment is essential in the context of decision-making [43]. As we have previously discussed, the number of paths grows exponentially with the size of the system. What is more, number of paths required to obtain reasonable coverage of total emissions Number of required paths depends strongly on the system under investigation [45].

In Panel A of Fig. 6, we show that for the simple case of a single-region input-output table of only 114 sectors, computation on current high-end consumer hardware may for some sectors take $2hrs$ while covering only 50% of total emissions in the computed paths. While is evident that for some sectors the structural path analysis does indeed converge quickly, for others the convergence behavior is very poor. Even computational optimizations such as parallelization cannot compensate for poor convergence behavior. In Panel B of Fig. 6 on the other hand, we show that the exact solution of a hybrid system system combining Ecoinvent and the Exiobase multi-regional input-output table of a combined 30’800 rows/columns can be computed exactly within $\sim 3min$ on the same hardware. For these solutions, we found excellent numerical stability to within floating-point precision for all calculations. The use of a path-based method, such as the path-exchange method, therefore confers no computational advantage.

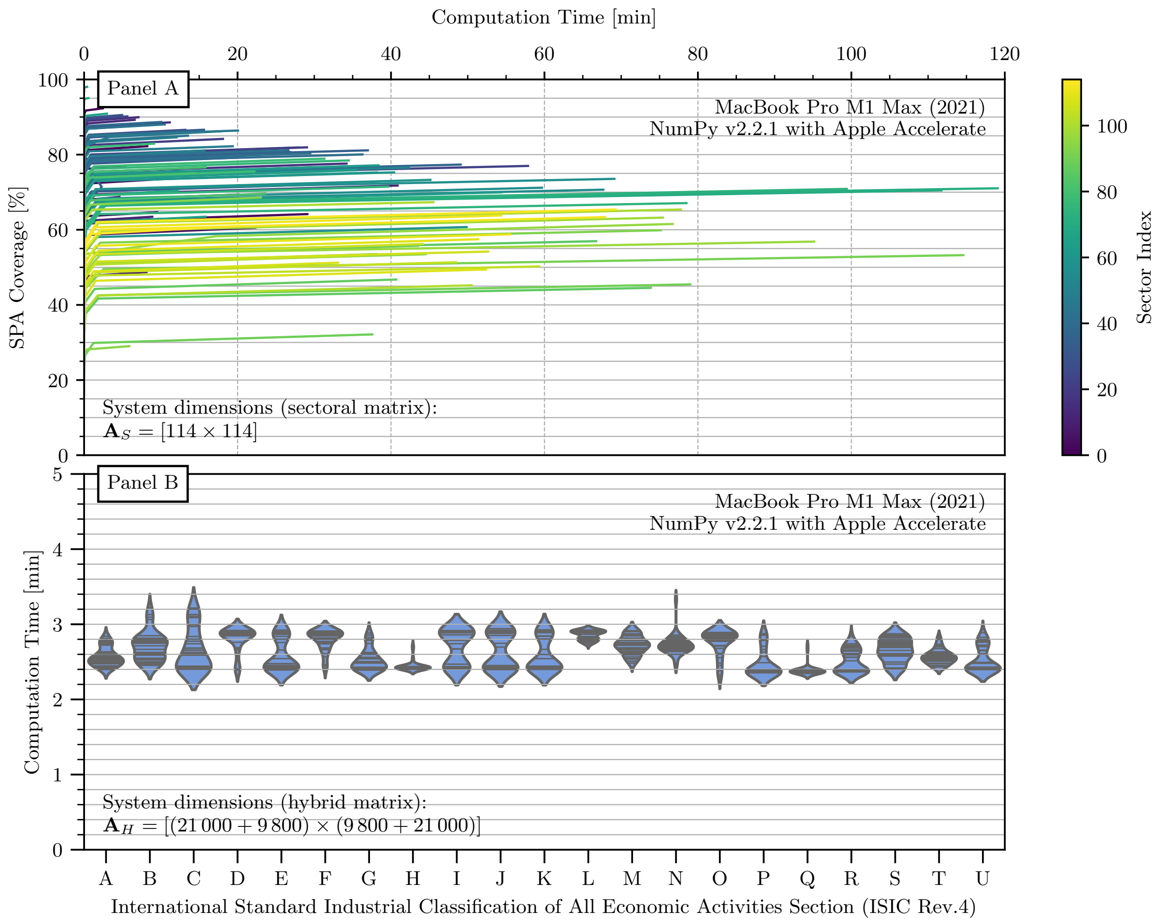

Figure 6: Computational intensity of the path-exchange (graph-based) hybrid life-cycle method and the tiered (matrix-based) life hybrid life-cycle method. *Panel A*: Convergence behavior of the environmental burden coverage from a structural path analysis for every sector in the input-output table of Australia. Every line represents a single sector. The maximum path length was set to 20, with the cut-off criteria varied between [0.1%, 0.01%, 0.001%, 0.0001%, 0.00001%]. In general, high SPA coverage in short computation time is desirable. It is evident that the convergence behavior strongly depends on the sector and can vary between $> 90\%$ in $\sim 5min$ to $< 50\%$ in $\sim 2hrs$ on current hardware. Note that this system is two orders of magnitude smaller than the hybrid system of Panel B. Computations were preformed using the `pyspa` [52] package (v2.4) on a MacBook Pro with an M1 Max CPU and NumPy (v2.2.1). *Panel B*: Computation time for the solution of the governing equation of hybrid life-cycle assessment $e = \mathbf{Q}_H \cdot \mathbf{B}_H \cdot \mathbf{A}_H^{-1} \cdot \vec{f}$ using the `numpy.linalg.solve(a,b)` function. The hybrid matrix was constructed by combining the Ecoinvent technosphere matrix of $\dim(\mathbf{A}_P) = [21'000 \times 21'000]$ and the multi-regional input-output table of the Exiobase 3 database [53] of $\dim(\mathbf{A}_S) = [9'800 \times 9'800]$. A sample of 10 Ecoinvent processes per ISIC section (A-U) was selected at random to serve as final demand. The numerical stability of every solution was checked by repeating the same computation 4 times. For every computation, the solution was found to be stable within the precision of the standard NumPy floating point data type. Note that this system is two orders of magnitude larger than the single-region input-output table of Panel A. Computations were preformed using NumPy v2.2.1. built against the Apple Accelerate BLAS framework on a MacBook Pro with an M1 Max CPU. All underlying data is available in a Zenodo repository [54].

7 Discussion

In Section 3.2, we provide a description of the path-exchange method supported by our novel diagrammatic notation introduced in Fig. 1. Following a short historical overview in Section 3.2, we show in Section 3.3 that the key assumption underlying the motivation for the development of the algorithm was incorrect. In Eq. (49) of Section 3.5 we then provide a concise mathematical description of the path-exchange method [10][11][28] for hybrid life-cycle assessment. This description makes use of a concordance matrix and the Iverson bracket. To our knowledge, no such definition has been provided to date. In order to augment the original visual illustrations of the algorithm provided by the authors in [11, Figure 2] and [28, Figure 1], a novel diagrammatic illustration is provided in Fig. 3. Finally, in Section 4 we show that the path-exchange (=graph-based) method for hybrid life-cycle assessment is mathematically equivalent to the tiered hybrid (=matrix-based) method for hybrid life-cycle assessment. The core of the proof is straightforward: A structural path analysis of the hybrid matrix compiled according to the tiered hybrid method is performed. Splitting up the indices of the matrix multiplication in the power-series expansion, it then becomes clear that the resulting paths are equivalent to those of the path-exchange method. An explicit example based on the system illustrated in Fig. 1 is provided in Section 5.

From Section 3.3 and Section 4, we can see that the frequently invoked argument of the path-exchange method working on *"mutually exclusive paths"* [11][28] is not an inherent property of the method. Instead it is a result of the algorithm making implicit use of binary double-counting correction. By extension, the claim that the method somehow avoids the problem of double-counting [14, Sec. 2.6.3][4, Table 4] is insubstantial. The method avoids instances of double-counting only through its implicit use of binary double counting correction. Finally, we can see that the purported advantage of avoiding *(...) the need to collect data and make assumptions that would be needed to populate the so-called upstream and downstream cut-off matrices (...) [which] makes the process more efficient as only the most significant nodes are modified."* [28, Sec. 2.1] is void: Downstream cut-off coefficients are not considered simply by definition of the path-exchange method algorithm. On the other hand, all information which the practitioner of the path-exchange method has on specific processes can easily be arranged into a matrix - the upstream cut-off matrix.

8 Conclusion

Ultimately, practitioners should be acutely aware of the inherent limitations of the path-exchange method we discuss in Section 3.4 and Section 6. While we have shown the tiered hybrid method and the path-exchange hybrid methods to be equivalent *in principle*, this holds true only in the case where the power series expansion of Eq. (49) is considered *ad infinitum* - a practical impossibility. We therefore suggest that the use of the former method is more prudent, since it avoids all these limitations by definition. This use of a matrix-based hybrid life-cycle assessment method should be preferred by practitioners, even in the case where individual paths are of interest, rather than just numerical value of the environmental burden. This is because a matrix method can also capture modifications at specific locations in the supply chain - and is computationally superior. If required, a structural path analysis can always be conducted on the tiered hybrid matrix, as we have shown in Section 4. This allows practitioners to determine the supply chain nodes with the highest overall environmental impact.

We hope that our formal treatment of the path-exchange method will provide some much-needed clarity in the ongoing discussion surrounding the specific properties and applicability of methods for hybrid life-cycle assessment. It is our hope that work toward a unified theory of methods will continue, ultimately providing a sound mathematical for the development of open-source tools, which can be integrated into mainstream software for life-cycle assessment.

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10 Code Availability

The source code used for generating the data visualized in panels A and B of Fig. 6 is available under a permissive license from a Zenodo repository [54].

11 Data Availability Statement

Part of the data that support the findings of this study are openly available, with links provided in a Zenodo repository [54]. Part of the data that support the findings of this study are available from Ecoinvent. Restrictions apply to the availability of these data, which were used under license for this study.

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