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The Virtual IELab – an exercise in replicating part of the EXIOBASE V.2 production pipeline in a virtual laboratory

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ABSTRACT
We explore options to replicate the EXIOBASE2 multi-region input–output (MRIO) database in the Virtual IELab cloud-computing laboratory environment. Whereas EXIOBASE2 is constructed using a multi-process reconciliation procedure, we present an alternative compilation technique that uses EXIOBASE2's pre-processed data and final tables in reconciling the IELab MRIO with conflicting raw data information. This approach skips the labour-intensive step of detailing and harmonising country tables. Adherence metrics reveal the EXIOBASE2-based IELab table to be considerably less balanced than the original but with stronger adherence to other constraints data. However, these metrics are not comparable to the original EXIOBASE2 statistics due to the distinctive implementation of constraint sets in the two platforms. IELab's main value-added is its flexibility in tailoring EXIOBASE2-based MRIOs beyond the original recipe. Finally, IELab's global carbon, water and material footprints are shown to be comparable with previously reported resource footprints. In contrast, deviations in land footprints warrant further investigation.

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International trade; multi-region input–output tables; EXIOBASE; virtual laboratory; global footprints

1. Introduction

The global interconnectedness we experience today has ushered in rapid economic growth, scientific innovations, technological advancements and many more improvements enhancing the overall quality of life. However, this new world order has detrimentally impacted the environment, placing stress on natural resources, and has given rise to a whole new set of socio-economic issues (e.g. see Lenzen et al., 2012a, 2012b; Alsamawi et al., 2014; Kanemoto et al., 2014; Oita et al., 2016; Tukker et al., 2016). Against this backdrop, there is increasing demand for understanding and assessing the implications of this phenomenon of global interconnection. National and multilateral statistical agencies have been embarking on data collection initiatives in response to this (see Tukker and Dietzenbacher, 2013).

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Nonetheless, these initiatives are not necessarily coordinated (Wiedmann et al., 2011; Inomata and Owen, 2014). This emphasises the pivotal role played by organisations that compile global multi-region input–output (MRIO) databases in harmonising and arranging data from different sources while following their respective philosophies and objectives. The massive databases they create serve as tools for enabling a better understanding of the various impacts of the ever-evolving world economic setup.

The overview article of this Special Issue by Lenzen et al. (2017) details the endeavour of researchers from different organisations that traditionally operate independently, to create a Global MRIO Virtual Laboratory, thereby taking advantage of economies of scale, avoiding replication and providing flexibility in building global MRIO tables. The Global MRIO Lab brings together some of the most prominent large-scale global MRIO frameworks in a cloud-based research platform suitable for implementing environmental and socio-economic modelling, essential for performing policy-informing studies. With the combined strengths of the major global MRIOs in one platform, the virtual laboratory (VL) provides a venue for undertaking studies aimed at shedding light on wellbeing and sustainability issues such as achieving a circular or green economy and enabling sustainable supply chains, among others (Wiedmann, 2017).

Results from numerous studies using MRIO-based analyses have contributed to public discussions and debates, especially on climate change (e.g. see Hertwich and Peters, 2009; Minx et al., 2009; Wiedmann and Barrett, 2013) and resource utilisation (e.g. see Wood et al., 2009; Daniels et al., 2011; Wiedmann et al., 2013; Giljum et al., 2016; Tukker et al., 2016; Verones et al., 2017). Generally, MRIO analyses allow assessment of trans-boundary impacts of consumption not only on the environment but also in terms of social implications (e.g. see Alsamawi et al., 2014; Simas et al., 2014; Reyes et al., in press). Thus, better consistency in compiling MRIO databases is of prime importance to enable understanding of pressing world issues and to identify hotspots for intervention.

Among the well-known world input–output datasets are the Asian International Input–Output Table (AIIOT)[1] by the IDE-JETRO (Meng et al., 2012), Eora[2] by the University of Sydney (Lenzen et al., 2012a, 2012b; 2013), the EU-funded EXIOBASE[3] (Tukker et al., 2013; Wood et al., 2015), GTAP9 Database[4] of the Global Trade Analysis Project (Andrew and Peters, 2013) and the World Input–Output Database (WIOD)[5] of the University of Groningen (Dietzenbacher et al., 2013). None of these databases are identical yet no single one can be considered superior to the others. Geschke et al. (2014) list possible reasons for this divergence: variation in classifications and levels of aggregation, differences in initial assembly and techniques used for reconciliation, and differences in source data. At large, it is as if different groups that compile MRIO tables use the same basic ingredients but follow different recipe books. More importantly, these differences also carry over to the quantification of impacts calculated using alternative MRIO frameworks. For instance, Owen et al. (2014) attribute the differences in consumption-based emissions computed using MRIO databases Eora, GTAP and WIOD to the dissimilarities in their Leontief

1 http://www.ide.go.jp
2 http://www.worldmrio.com
3 http://www.exiobase.eu
4 https://www.gtap.agecon.purdue.edu
5 http://www.wiod.org/new_site/home.htm

inverses, final demand and emissions data. Additionally, despite harmonising the carbon satellite accounts of Eora, WIOD, EXIOBASE and the GTAP-based OpenEU MRIOs, Moran and Wood (2014) still find differences in the order of $< 10\%$ when calculating the carbon footprint of major economies.

Inomata and Owen (2014) recommend that to tackle the divergence in MRIO systems, users would have to be forthright in dealing with uncertainties, and discuss the implications of their choice of data sources and construction techniques on the results of their analysis. Indeed, over a short time period, several developments have occurred in the field of global MRIO of which the origins and historical account are traced in Tukker and Dietzenbacher (2013). A 'single global MRIO maintained and regularly updated by one institute (perhaps in collaboration with others)', an option entertained by Peters and Solli (2010, p. 109) and reiterated by Wiedmann et al. (2011) on their discussion of the role of automation in data compilation, may not be fully realised yet, but this vision of The Project Réunion[6] is taking shape in the form of the Global MRIO Lab.

2. Motivation

This work aims to contribute to the vision of Project Réunion by demonstrating the possibility of incorporating one of the major world input–output databases, EXIOBASE, to the collaborative VL environment offered by the Virtual Industrial Ecology Lab (Lenzen et al., 2014). Lenzen et al. (2017) provides a detailed discussion of the overarching rationale driving this project along with the potential benefits to the research community of advancing collaborative work on MRIO compilation.

The EXIOBASE database is extremely helpful in providing insights on how consumption drives environmental and socio-economic pressures in different territories (e.g. see Tukker et al., 2014; 2016; Simas et al., 2014; Wood et al., 2015; Giljum et al., 2016). Analyses based on such databases are essential in the effective pursuit of key sustainability agendas. Specifically, EXIOBASE specialises in providing the highest resolution of details for the agriculture, energy and waste sectors where environmental and resource impacts are most relevant, with its main focus on Europe and other major economies (Wood et al., 2014). None of the existing MRIO databases can rival the level of detail it offers on environmental- and resource-related sectors. These characteristics make it an ideal input to the laboratory environment, allowing the exploration of alternative options of reconstruction, namely a less user-intensive input process in a highly automated setting.

EXIOBASE leverages its strength of offering detailed harmonised product and industry classifications of global trade transactions. Because of its complex production process, it contains more interindustry detail compared to most official country supply-use tables (SUTs). In particular, EXIOBASE version 2 (EXIOBASE2) is constructed in two major steps. First, country tables are detailed using a number of auxiliary data, harmonised into a high-resolution common classification, and balanced individually. This labour-intensive step involves considerable pre-processing of data. Second, the detailed country tables are linked via trade. Since global trade statistics including imports and exports in country

[6] The Project Réunion consortium is the result of a small-scale workshop held in the Island of Réunion of representatives of major institutions involved in the compilation of global MRIO databases, following the 18th Input–Output Conference held in 2010 at the University of Sydney, that originated the idea of global research collaboration for harmonising activities and enhancing synergy and efficiency on MRIO compilation. (http://www.isa.org.usyd.edu.au/mrio/mrio.shtml)

SUT/input–output table (IOT) are not balanced, adjustments of country SUTs and IOTs are necessary to obtain balanced global table flows.

This sets the stage for exploring adoption of an alternative construction procedure in the Lab environment that does not repeat the labour-intensive detailing exercise. This can be achieved using the existing sectorally detailed EXIOBASE2 database as an input, and globally balancing and reconciling the MRIO with auxiliary source data in a single-step optimisation procedure. Moreover, with the Virtual IELab, users gain flexibility in choosing adherence to specific raw data sets, as opposed to the original EXIOBASE2 MRIO which uses a single specific recipe. However, recreating an alternative version of EXIOBASE2 in the IELab hinges on the availability of the EXIOBASE2 data, without which as the starting point, this exercise would not be possible in the first place.

Taking steps towards bringing EXIOBASE to a common platform with other prominent MRIO databases paves the way for combining the best features of various MRIO databases in the future. This presents new opportunities for further improving the MRIO compilation process, the quality of the compiled tables, and, consequently, the analyses arising from them. In the VL, the collaborative research platform also allows sharing of data repositories and computational tools, including visualisation and uncertainty reports.

This article describes the implementation of EXIOBASE2 in the Virtual IELab and compares the contingency tables compiled by the Lab vis-à-vis the original EXIOBASE2 MRIO tables. Finally, global carbon, water, land and material footprints are calculated in the IELab to illustrate the effect of the alternative MRIO construction procedure and specifications in the Lab on outcomes of IO-based analysis, even where the same underlying data were used for table compilation.

3. Data

As agreed upon between The Project Réunion and the EXIOBASE consortium, for this proof of concept exercise, part of the EXIOBASE production pipeline is replicated in the Virtual IELab using the full EXIOBASE2 dataset which includes both its final monetary table and its other data sources. EXIOBASE2 is the second version of the global, detailed multiregional environmentally extended supply and use/input–output (MR EE SUT/IOT) database for year 2007, constructed by the EXIOBASE team in the CREEA[7] project (Wood et al., 2015). This reflects improvements to EXIOBASE's first version (EXIOBASE1) developed within the EXIOPOL project (Tukker et al., 2013), elaborated to ensure consistency with the United Nations' standard on the System of Environmental-Economic Accounting (SEEA) 2012 (United Nations, 2017). EXIOBASE2 expands the EXIOBASE coverage to 43 countries and five rest of the world (RoW) regions, 200 products, 163 industries, 15 land use types, three employment skill levels, 48 types of raw materials and 172 types of water use. At the time of writing, EXIOBASE is being revised as a time series database spanning the years 1995–2011 under the DESIRE[8] project (Wood et al., 2015; Stadler et al., 2017).

EXIOBASE2 offers the most detailed homogeneous product and industry classification with respect to agriculture, resource extraction and electricity generation and traces waste and recycling flows that are not typically available in other MRIO databases. Its SUTs are

[7] CREEA is the acronym for Compiling and Refining of Economic and Environmental Accounts.
[8] DESIRE is the acronym for Development of a System of Indicators for a Resource efficient Europe.

presented in a rectangular instead of square format allowing representation of a single technology that produces more than one product or multiple co-products (Wood et al., 2014; 2015). The disaggregation to such a level of sectoral detail requires a high degree of data interrogation and a number of raw datasets from different sources.

The various data used in building EXIOBASE2, also employed in constructing the IELab version in this study, are listed below. Detailed discussions on these data sources, including their processing and use by the EXIOBASE team, can be found in Tukker et al. (2013) and Wood et al. (2015).

(a) National Account (SUT) data such as the European System of Accounts of 1995 (ESA95) SUTs comprising 59 sectors and products for 27 European Union member states as of 2007 (EU27)[9] and SUT and/or IO table in varying classifications for the 16 non-EU countries.
(b) Agriculture Social Accounting Matrices (AgroSAM) for the EU27 with disaggregated agricultural data for 30 primary agricultural sectors and 11 food processing sectors.
(c) Agricultural Production Output (AgriProd) based on Food and Agriculture Organisation of the United Nations Statistics (FAOSTAT) coupled with AgroSAM data for agricultural sector production values.
(d) Production Communautaire database (PRODCOM) for manufacturing product output for European countries.
(e) Structural Business Statistics (SBS) for data on industry turnover.
(f) International Energy Agency (IEA) Energy Balance database plus price and tax data for conversion to monetary units.
(g) United Nations Industrial Development Organisation (UNIDO IndStat) Industry Statistics database for other production data.
(h) International Trade Database (Base pour l'Analyse du Commerce International, BACI) based on United Nations Commodity Trade Statistics Database (UN Comtrade) for reconciled trade flow data.

Finally, the physical satellite data on carbon dioxide-equivalent (CO2-eq) global warming potential (GWP), volume of blue water consumption (surface and ground water withdrawals), land use and raw material consumption (RMC) from EXIOBASE2 are imported into the IELab to enable footprint calculations.

4. Methods

4.1. IELab procedure for implementing the EXIOBASE2 production pipeline

EXIOBASE2, as constructed by the EXIOBASE team, uses a multi-process reconciliation procedure, which can be broken down into two somewhat distinct steps. First, country tables from National Statistical Institutes (NSIs) are detailed and harmonised into a common conceptual framework and a homogeneous classification of a higher resolution than offered by most NSIs. The workflow follows a sequential order on the use of auxiliary data

[9] EU27 includes member states Austria, Belgium, Bulgaria, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, the Netherlands, Poland, Portugal, Romania, Slovak Republic, Slovenia, Spain, Sweden and the United Kingdom.

from FAO and the European AgroSAM for agriculture, the IEA database for energy carriers and electricity, various resource databases, other related datasets, and representative coefficient estimates incorporating physical data for the cell-by-cell disaggregation that disturbs the production balances across supply, use and auxiliary data (Tukker et al., 2013). This necessitates the first balancing step in order to ensure the tables remain balanced while adhering to aggregate SUT data after incorporating a higher level of detail in the transactions. Another procedure is carried out to estimate and detail the five RoW regions in the database (For the intricacies of this procedure, see Stadler et al., 2014).

Second, these detailed country tables are linked via trade. The trade-linking procedure comprises disaggregation of import use tables, allocating imports to countries of exports using UN Comtrade trade shares, tackling the resulting implicit exports with exports in the SUT, and performing another balancing step to adjust for these differences (Tukker et al., 2013; Bouwmeester, 2014; Wood et al., 2015). The EXIOBASE consortium also estimates physical extensions or satellite accounts, especially the environmentally significant ones, and augments them to match the monetary accounts. The final stage of the wokflow is the importation of all data in the EXIOBASE database system.

In the IELab workflow, a simplified approach of the above is employed. We do not attempt to replicate the first, labour-intensive reconciliation step for creating the detailed country tables. Rather, we use EXIOBASE2 as input in an alternative mathematical reconciliation technique that balances trade and auxiliary source data. This creates an alternative version of EXIOBASE2 that is part of the Global MRIO Lab with a similar architecture to that of its predecessor, the Australian IELab, described in Lenzen et al. (2014, 2017). The construction workflow involves (a) specifying the initial estimate (IE) for interindustry interregional transactions, final demand and value-added matrices, based on available EXIOBASE2 data, in this case, (b) detailing a set of constraints on values and relationships that the elements in the compiled MRIO table must adhere to, (c) reconciling the IE with conflicting sets of constraining information handled by the KRAS optimisation engine in AISHA[10] (Geschke et al., 2011) and (d) generating the desired MRIO table with which IO-based analyses can be conducted. These steps are a simplification of the more complicated EXIOBASE workflow. This work is an adaptation of a previous work by Geschke et al. (2014) for the Lab environment.

4.1.1. Initial estimate

A critical ingredient in MRIO compilation is a high quality IE. Geschke et al.'s (2014) investigation on how the different parts of an MRIO construction process influence the quality of the final MRIO finds that better IEs yield MRIOs with stronger adherence to constraint data. It is therefore important to specify an IE of superior quality. Without such a database as the starting point, applying even the most sophisticated estimation procedures on the data may yield an MRIO with reliability issues. In this proof of concept work, we select the monetary data of the final version of the EXIOBASE2 database as the IE of the intermediate demand, final demand and value-added matrices for building the IELab. Thus, the structure of the tables compiled with the IELab relies heavily on that of the final EXIOBASE2 database.

[10] AISHA, an acronym for An Automated Integration System for Harmonised Accounts, is a MATLAB-based tool for constructing large contingency tables developed at the University of Sydney and is the system adopted for the Global MRIO Lab.

Ideally, an IE is built by putting together raw data from various sources, requiring a great deal of data pre-processing. For instance, for the construction of EXIOBASE1 in the EXIOPOL project (Tukker et al., 2013; Wood et al., 2014), and later the construction of EXIOBASE2 (Wood et al., 2015), the EXIOBASE consortium devoted significant time on quality controlling the data pre-processing, for example, on the proper treatment of purchases by residents abroad, the handling of taxation layers, the disaggregation of the original SUT of a country from 59 industries and products to 163 industries and 200 product categories using relative shares from auxiliary data sources, listed in Section 3 as *b* to *g*, among others. While this construction process is largely automated and updates of country tables can be made with much less time, duplicating this procedure to build the IE in the context of the Global MRIO Lab would be very laborious. As highlighted in Lenzen et al. (2017) in this Special Issue, compromises are inevitable in the pursuit of the Global MRIO Lab project (Lenzen et al., 2017).

It is important to note that the IE of the IELab database must be in the full EXIOBASE level of disaggregation. In order to feed this into the VL, the EXIOBASE2 classification is therefore used as the root classification[11] for the Virtual IELab version of EXIOBASE2. The IE feed, written as a processing script, slots the EXIOBASE2 tables to IELab MRIO format presented in Section 4.1.4.

4.1.2. Constraints

The Lab is designed to improve efficiency in MRIO compilation by allowing sharing of resources including data and constraint feeds that can be reused in the Global MRIO Lab platform for building user-specific tables. For this purpose, data feeds[12] for the EXIOBASE2 constraints data set from Geschke et al.'s (2014) investigation on mixing compilation pipeline elements are tapped and modified to suit the Lab environment.

Constraints are defined in the Lab to ensure that the elements of the compiled MRIO table take values consistent with raw data information and relationships whilst obeying the MRIO structure principles. Geschke et al. (2011; 2014) explain the details of how constraints are expressed in AISHA language or A-LANG form, which can be parsed by IELab's underlying computational system. In this case, eleven processing scripts comprising eight constraint feeds that correspond to the eight raw data sources used in EXIOBASE2 compilation, listed in Section 3, along with three balancing constraint feeds are used for constructing the EXIOBASE2-based IELab.

Whilst the EXIOBASE2 SUTs use a non-overlapping set of constraints that cover the supply and use tables,[13] the IELab version more easily uses overlapping constraints even when conflicts occur, as constraint reconciliation is built into the optimisation procedure (compare Wood et al., 2009; 2014). This has advantages in that conflicting data do not need to be pre-reconciled and that confidential data can be estimated as part of the procedure. In the IELab, the national SUTs are translated to 330,860 point or absolute constraints,

[11] The root classification refers to the maximum sectoral and spatial disaggregation of the MRIO that provides the highest level of details (Lenzen et al., 2017).

[12] Data feeds are purpose-built pieces of code that are used to convert raw data into a format which the MRIOLab suite can process in a fully automated way (Lenzen et al., 2017).

[13] This is to avoid discrepancies between disaggregate and aggregate constraints, such as row totals, that might occur in the official SUTs.

which is roughly 10% more than the constraints in the EXIOBASE2 procedure because of the inclusion of aggregate totals. Hence during reconciliation, the elements of the IELab-compiled table are specified to take values as close as possible to the values in these original SUTs in their native classification, which may have fewer or more sectors than the root classification.

The auxiliary data used by the EXIOBASE team for detailing the SUTs to the homogeneous 163 industries and 200 product categories, such as the AgroSAM, AgriProd, PRODCOM, SBS, IEA and UNIDO IndStat, are converted to ratio constraints. The ratio constraints confront the MRIO elements to preserve the ratios dictated by the values in the source data. Thus, a total of 351,424 AgroSAM ratio constraints, 789 AgriProd ratio constraints, 1456 PRODCOM ratio constraints, 1236 SBS ratio constraints, 8942 IEA ratio constraints and 910 UNIDO IndStat ratio constraints are fed into IELab. If in EXIOBASE2's multi-step balancing workflow, discussed previously, the trade-linking step is performed separately using trade data, in IELab, the reconciled BACI trade flow data are treated the same way as the foregoing auxiliary data and transformed to 281,200 ratio constraints. Hence, these proportions from all seven databases are simultaneously respected during reconciliation.

The last set of constraints utilised for the IELab (17,424 in total) is for balancing industry and product totals; balancing the margin sheets of taxes less subsidies, trade margin and transport margin; and setting boundary values, like non-negativity constraints for most of the elements and as appropriate for others.

The constraint feeds also specify the standard deviation tag for every data source or constraint depending on known or perceived data reliability of the source as well as on the objectives and philosophies guiding the user. It is possible to tighten or loosen the degree by which data points are allowed to vary during reconciliation. For instance, one can assign a specific value of 0.1% or 10% or a range of values like the maximum value in the data set being allowed to have a relative standard deviation of 0.01% or 1%, and the smallest value a standard deviation of 0.3% or 30%.

4.1.3. Reconciliation

Instead of the multi-step balancing procedure employed in constructing EXIOBASE2, we streamline the compilation workflow in IELab to a single-step mathematical reconciliation technique using the VL's high-performance computing capability. Consistent with Geschke et al. (2011; 2014), the problem solved in the optimisation procedure is as follows. A penalty objective function is minimised to find the final EXIOBASE2-based IELab MRIO (vectorised as p_1) with minimal departure from the IE (vectorised as p_0) subject to the final MRIO adhering to all constraints defined by the superior data ($Gp_1 = c$, where $\mathbf{G}$ is the matrix of coefficients connecting raw data to elements of the MRIO and $\mathbf{c}$ is the vector of constraints representing the raw data) and boundary conditions described in the previous section. This means the EXIOBASE2 database which serves as the IE is reconciled in one step with the SUT point constraints, auxiliary and BACI trade ratio constraints, and balancing constraints in order to compile the IELab version. The auxiliary data such as AgroSAM and IEA (used for the SUT detailing step in the EXIOBASE2 workflow) and the original country SUTs used in the trade-linking step (where the detailed SUTs are combined with BACI trade information) are not revisited. Instead, the IELab builds the final MRIO by using the EXIOBASE2 final database, all raw data information from the two main steps of EXIOBASE2 workflow as constraints, and the required relationships among MRIO table elements as the ingredients in one optimisation procedure.

It is likely that the numerous constraints embody conflicting information. These conflicting sets of constraining information are addressed by the KRAS optimisation technique used in the Lab by incorporating in the solution reliability information of raw data given as standard deviation tags on the individual data points. The standard deviations are estimated following the approach proposed by Lenzen et al. (2009). Discussion on the merits of the KRAS balancing procedure can also be found in Lenzen et al. (2009).

4.1.4. The IELab version of the EXIOBASE MRIO

The original publicly available EXIOBASE2 database consists of a condensed rectangular product-by-industry supply table and use table with 9600 rows and 7824 columns a final demand table with 9600 products and 7 final demand types for 48 regions, and factor inputs table with 19 factor input types for 7824 industries, with their representations shown on the upper panel of Figure 1. The compiled IELab database, on the other hand, takes the MRIO form shown on the lower panel of the same figure. Here, the principal diagonal of the transactions matrix contains the domestic supply and domestic use blocks, and the off-diagonals contain the import use blocks. The final demand and value-added or factor inputs matrices are arranged to suit the format of the transactions matrix. IELab assembles a $17,424 \times 17,424$ intermediate demand table, a $17,424 \times 336$ final demand table and a $912 \times 17,424$ value-added table, the elements expressed in million Euros. These representations of EXIOBASE2 and the IELab, despite featuring different table arrangements, are equivalent.

The arrangement of submatrices in IELab format follows the Global MRIO Lab's system of organising contingency tables with elements of each country's transactions matrix grouped together. Like in EXIOBASE2, in the IELab the multi-regional table is compiled in multi-region SUT format, making it convenient for performing impact analysis in the form of multipliers and footprints, without the limitations associated with the use of symmetric IOTs (Rueda-Cantuche, 2011; Lenzen and Rueda-Cantuche, 2012). A drawback of this is the fact that it doubles the size of the final analytical table without additional information (Rodrigues et al., 2016).

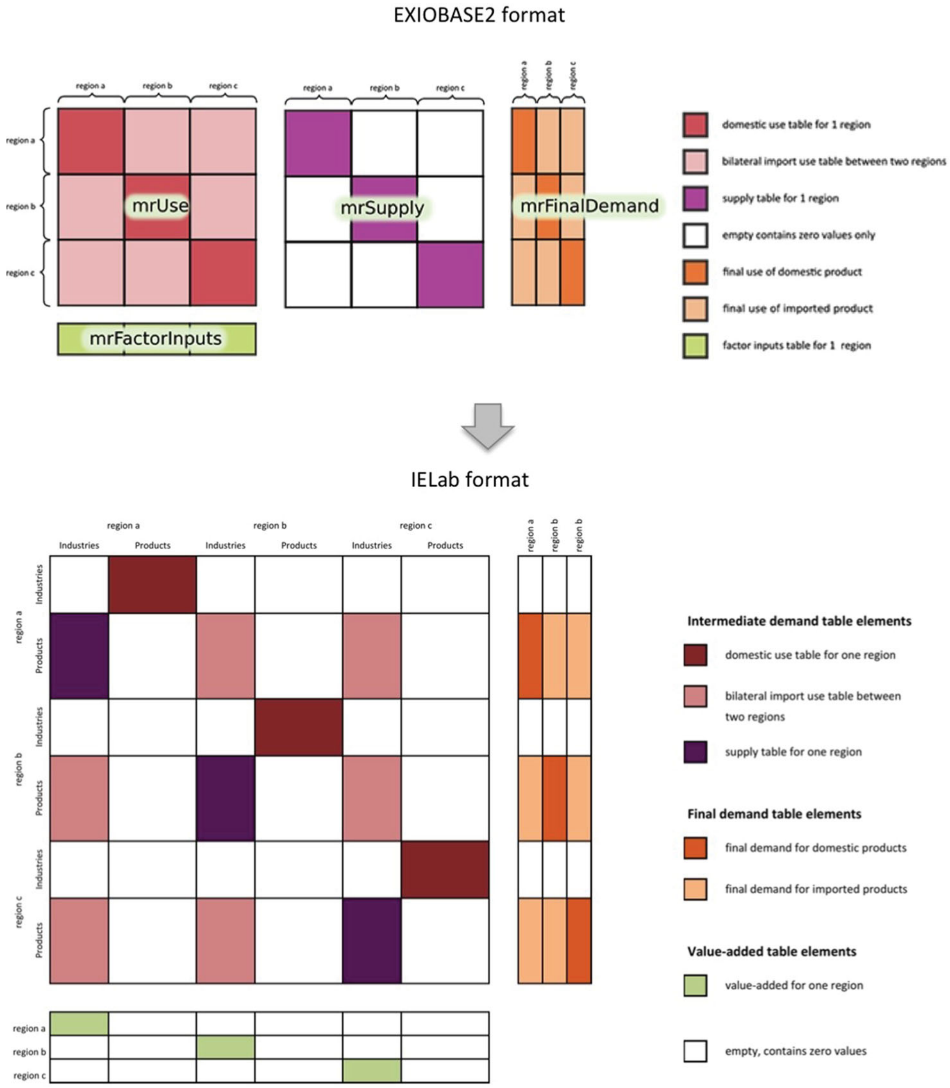
4.2. Matrix distances and test of adherence

To perform a comparison between the EXIOBASE2 database and the IELab contingency tables, as well as their adherence to source data, matrix distance metrics are used. The distance measures utilised in this work are the mean absolute difference (MAD), RAS-type entropy (RAS-E), root mean squared error (RMSE), equivalently the Euclidean metric distance (EMD), and the complement of the correlation coefficient (DCORR). Suppose matrices **A** and **B** with equal dimensions $m \times n$ are compared, then the distance norms are calculated as follows:

Mean Absolute Difference (MAD) (Lahr, 1998):

$$\frac{\sum_j \sum_i |a_{ij} - b_{ij}|}{mn} \tag{1}$$

Figure 1. Schematic of the IELab MRIO format based on EXIOBASE2.



Note: The figure on the upper panel is reproduced with minor adjustments from Tukker et al. (2014; 2016) and can also be found at http://www.exiobase.eu/index.php/2-uncategorised/29-exiobase2-mr-sut.

RAS-type Entropy (RAS-E) (Knudsen and Fotheringham, 1986):

$$\sum_j \sum_i p_{ij} \ln \left(\frac{p_{ij}}{q_{ij}} \right) \tag{2}$$

$$\text{where } p_{ij} = \frac{b_{ij}}{\sum_j \sum_i b_{ij}} \text{ and } q_{ij} = \frac{a_{ij}}{\sum_j \sum_i a_{ij}}$$

Euclidean Metric Distance (EMD)/RMSE (Lahr, 1998):

$$\frac{\sqrt{\sum_j \sum_i (a_{ij} - b_{ij})^2}}{mn} \tag{3}$$

Complement of Pearson's Correlation Coefficient (DCORR) (Lahr, 1998):

$$1 - \frac{\sum_j \sum_i (a_{ij} - \bar{a})(b_{ij} - \bar{b})}{\sqrt{\sum_j \sum_i (a_{ij} - \bar{a})^2} \sqrt{\sum_j \sum_i (b_{ij} - \bar{b})^2}} \tag{4}$$

Distance metrics MAD, EMD/RMSE and DCORR are selected based on Wiebe and Lenzen's (2016) review of matrix comparison techniques.[14] These metrics have also been previously used by Geschke et al. (2014), Owen (2015), Wood (2011), and Wood and Lenzen (2009) for comparing databases. With a lower bound of 0, smaller values of MAD and EMD indicate smaller differences between the matrices compared. In contrast, the correlation coefficient is a measure of association or similarity bounded by −1 and 1, signifying perfect negative correlation and perfect positive correlation, respectively, while 0 indicates no correlation. It is converted to a divergence metric by taking its complement with 1 as DCORR. For matrices that are positively correlated, a DCORR value closer to 0 exhibits less differences and a value closer to 1 shows greater distance. The RAS-E is added to the suite of relevant norms to measure information loss. This metric is especially appropriate in this work since the KRAS optimiser used in the IELab reconciliation minimises a RAS-type minimum-information objective function (Lenzen et al., 2009).

The four norms above are used for comparing the intermediate demand, final demand and value-added matrices of EXIOBASE2 with the IELab-compiled tables, where **A** in the above formula corresponds to the particular EXIOBASE2 matrix under investigation and **B** is the IELab matrix. Similarly, tests of adherence to constraints are implemented by treating the constraints realisation of the IE $\mathbf{Gp}_0$ or constraints realisation of the IELab-compiled table $\mathbf{Gp}_1$ as matrix **A** and raw data **c** as matrix **B**, so that the norm $\mathbf{Gp}_0 - \mathbf{c}$ measures adherence of EXIOBASE2 to raw data, while $\mathbf{Gp}_1 - \mathbf{c}$ measures adherence of the IELab.

4.3. Footprint calculation

The analysis then proceeds to delving into the effect of alternative MRIO construction procedure and specifications in the Lab on outcomes of IO-based analyses despite the use of the same underlying data. This is carried out by analysing the differences of footprints computed using the original EXIOBASE2 vis-à-vis those from the IELab.

The footprint calculation uses conventional input–output model formulation as follows (Miller and Blair, 2009). Representing the equilibrium condition supply equals demand, total production **x**, a column vector with k elements, equals total demand, that is, the sum of intermediate or interindustry demand **T**, a $k \times k$ square matrix (k rows and k columns), and final demand **Y** of households, firms, the government and the rest of the world, a matrix

[14] A measure of goodness-of-fit, *R*-squared is among the typical metrics for comparing matrices. Although calculated, it is not presented in this work since it captures the same information as correlation, with R-squared equivalent to the square of the correlation coefficient in simple linear regression (Wiebe and Lenzen, 2016).

with $k \times r$ dimensions. In equation form, $\mathbf{x} = \mathbf{T1}^k + \mathbf{Y1}^r$ where $\mathbf{1}^k = \underbrace{\{1, 1, \ldots, 1\}}_{k \text{ elements}}$ and $\mathbf{1}^r = \underbrace{\{1, 1, \ldots, 1\}}_{r \text{ elements}}$ are the summation operators.

The direct requirements matrix holding the so-called production recipes of industries is calculated by taking the ratio of input to total output as $\mathbf{A} = \mathbf{T}\hat{\mathbf{x}}^{-1}$, equivalent to the expression $\mathbf{T1}^k = \mathbf{Ax}$. This brings us to the IO identity $\mathbf{x} = \mathbf{Ax} + \mathbf{Y1}^r$ with solution $\mathbf{x} = (\mathbf{I} - \mathbf{A})^{-1}\mathbf{Y1}^r = \mathbf{LY1}^r$, where $\mathbf{I}$ is a $k \times k$ identity matrix and $\mathbf{L} = (\mathbf{I} - \mathbf{A})^{-1}$, that is, the well-known Leontief inverse capturing both the direct and indirect input requirements for meeting a Euro of final demand.

Each physical satellite account $\mathbf{Q}$ is introduced as a row vector with k elements that can further be expressed in per Euro of output units as $\mathbf{q} = \mathbf{Q}\hat{\mathbf{x}}^{-1}$. In this work, the satellite accounts carbon, water, land and materials are analysed. The carbon, water, land and material footprints can then be computed using the equation $\mathbf{f} = \mathbf{qx} = \mathbf{qLY1}^r = \mathbf{mY1}^r$ with $\mathbf{m}$ multipliers that account for both the direct and embodied values of the indicator or satellite account referenced against a Euro of final demand, that is, per Euro spent on everyday consumption. The calculated footprint, represented by vector $\mathbf{f}$, hence expresses direct and embodied impacts associated with consumption across each economic sector.

5. Results and discussion

5.1. Matrix differences and adherence: EXIOBASE2 vis-à-vis IELab-compiled table

The calculated distance metrics for the intermediate demand, final demand and value-added matrices between EXIOBASE2 and an EXIOBASE2-based table compiled in the IELab are reported in Table 1. EXIOBASE2 tables are first arranged in IELab format so that these norms are computed on full IELab format as shown in the lower panel of Figure 1. The MAD and EMD between the IELab MRIO table and EXIOBASE2 are smallest for the intermediate demand and value-added tables and slightly larger for the final demand table. Across all tables, close to zero values of the DCORR signify extremely high degree of correlation of the two databases.

Apart from the level values of the MAD and EMD, proportions as compared to the norms of their respective EXIOBASE matrices are also reported to provide a more relative percentage of deviation. The intermediate demand may appear to have the lowest

Table 1. Differences between the IELab-compiled and EXIOBASE2 tables.

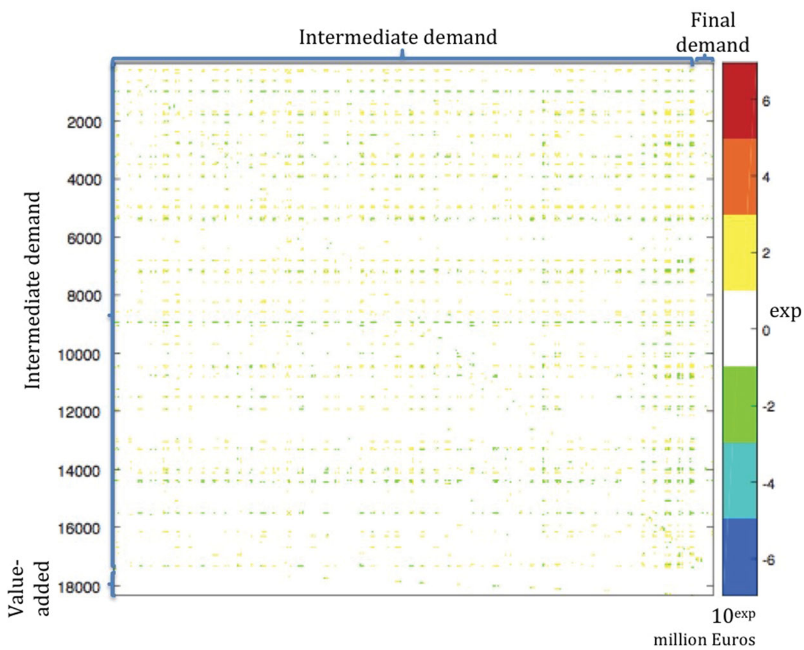
	MAD[a] (as % of IE MAD[b])	EMD[a] (as % of IE EMD[c])	DCORR
Intermediate demand table	0.042 (11%)	0.001 (8%)	0.004
Final demand table	0.697 (11%)	0.029 (6%)	0.002
Value-added table	0.043 (0%)	0.004 (0%)	0.000

[a]In million Euros.
[b]IE MAD is calculated as the MAD of EXIOBASE2 elements from its mean, $\sum_j \sum_i |a_{ij} - \bar{a}|/mn$.
[c]IE EMD is calculated as the EMD of EXIOBASE2 elements from its mean, $\sqrt{\sum_j \sum_i (a_{ij} - \bar{a})^2/mn}$.

MAD and EMD norms in the group, at 42 and one thousand Euros, respectively, and even lower than average of those from Geschke et al.'s (2014) comparison of intermediate demand matrices after mixing compilation pipeline elements of different MRIO databases. However, when viewed relative to the IE norms, the differences in intermediate demand across the two databases represent between 8% and 11% of the usual variation in the EXIOBASE table. The opposite is true for the value-added tables where the MAD and EMD values suggest a larger degree of variation, but as percentages of the IE norms, the distances between EXIOBASE2 from the IELab MRIO are revealed to be minimal and these value-added tables are, in fact, almost perfectly correlated with each other. The distance metrics for the final demand tables are the largest in magnitude with 6% to 11% deviation.

The heat map of the absolute differences between the two databases in Figure 2, also presented in IELab format, shows departures ranging from zero to 100 million Euros between EXIOBASE2 and IELab. The differences can be found in the elements that are supposed to be populated like the domestic supply and use blocks along the principal diagonal, the interregional use tables on the off-diagonal blocks, the final demand blocks on the right side column and the value-added blocks as a diagonal at the bottom of the heat map. The faint heat map attests to the minimal variation from EXIOBASE2 to IELab-compiled table when viewed at a macro level.

Figure 2. Heat map of differences between IELab-compiled and EXIOBASE2 databases (IELab – EXIOBASE2).



Notes: The positive numerical values on the legend represent the exponent of base 10, for example, 2 represents 10^2 = 100, 4 represents 10^4 = 10,000; the negative values represent the negative counterparts of the former, for example, −2 translates to −100, −4 translates to −10,000; and 0 still represents 0.

Table 2. EXIOBASE2 and IELab distances from constraint data by type, as implemented in the MRIO Lab.

			MAD		RAS-E		EMD		DCORR	
No. of constraints	SD tag	Constraint type	EXIOBASE2 $\lVert Gp_0 - c \rVert$	IELab $\lVert Gp_1 - c \rVert$	EXIOBASE2 $\lVert Gp_0 - c \rVert$	IELab $\lVert Gp_1 - c \rVert$	EXIOBASE2 $\lVert Gp_0 - c \rVert$	IELab $\lVert Gp_1 - c \rVert$	EXIOBASE2 $\lVert Gp_0 - c \rVert$	IELab $\lVert Gp_1 - c \rVert$
330,860	0	SUTs	32.01	29.86	0.017	0.013	1.11	0.92	0.002	0.001
351,424	0.1	AgroSAM	55.78	51.46			1.07	0.93		
789	0.1	AgriProd	1053.77	357.54			118.62	32.30		
1456	0.1	PRODCOM	1006.84	644.46			74.92	45.41		
1236	0.1	SBS	7369.79	6297.24			773.52	660.00		
8942	0.1	IEA	1062.87	209.10			63.29	11.17		
910	0.1	UNIDO	5053.42	3916.98			509.66	371.28		
281,200	0.1	BACI	19.11	7.26			0.49	0.12		
17,424	0.0	Balance	1.10	275.71			0.16	8.78		
994,241		Overall	61.45	49.53			1.34	1.01		

Note: Values that indicate better adherence to constraints are highlighted.

The adherence examination provides further insightful results. It appears that there is room for improving the adherence to source data with the Lab compilation of MRIO tables but not without a trade-off. Table 2 shows diagnostic test results for the EXIOBASE2 original database and the IELab, both as totals and sorted by constraint type. The overall consistency with raw data information is enhanced in the Lab version of EXIOBASE2 across all distance measures. This is based on a table compiled with nil standard deviation (SD) tag assigned to the SUT point constraints as well as to the balancing and boundary constraints, and 0.1 or 10% SD uniformly attached to the rest of the data sources.[15] The MAD, RAS-type entropy, EMD and the complement of the correlation coefficient norms are all lower in the IELab, in total (Table 2).

The most relevant norms in this study are the RAS-type entropy and the MAD. This is because the philosophy embraced by the Lab's contingency table construction includes minimisation of information loss and minimisation of constraint conflict. These objectives are addressed with the use of the KRAS optimiser for balancing and reconciliation. KRAS minimises a RAS-type minimum-information function whilst limiting the absolute distance between the constraints and their realisations, as in MAD, in conjunction with uncertainty information (Lenzen et al., 2009). Consistent with Oosterhaven (2005), the most appropriate value norms for evaluating performance are those that match the penalty or target function of the optimisation algorithm employed, although Strømman (2009) argues the benefits of multiple-objective functions. As shown in Table 2, the MAD to raw data decreases from 61 in EXIOBASE2 to 50 in the IELab while the RAS-type entropy falls marginally from 0.017 to 0.013, respectively.

An examination by constraint type using the applicable distance measures unveils improvement of adherence to SUTs, agriculture databases, PRODCOM and SBS manufacturing and industry data, IEA energy database, UNIDO industry statistics and BACI trade database constraints, all of which come at the cost of balancing. Note that EXIOBASE2 adheres 100% to the SUT constraints when disaggregation occurs, in contrast to the results presented here. The differences observed here are thus probably due to the overlapping constraint sets included in the IELab in comparison to EXIOBASE2, but further research is needed to substantiate this. What is evident in Table 2 is that, when viewed through the constraint relationships implemented in the IELab, EXIOBASE2 already adheres relatively well to the trade data and individual country SUTs, in addition to being better balanced. The optimisation in the IELab brings the MRIO elements closer to the SUT values and trade ratios of BACI. However, in the process, the balances are disturbed and the violations to the balancing constraints rise, as seen in an MAD increase of 274.6 and an EMD increase of 8.6 from EXIOBASE2 to the IELab.

Figure 3 illustrates MRIO adherence itemised by type of SUT and IEA data. The 16 rocket plots here show violations in EXIOBASE and IELab of the various detailed constraints, as implemented in the Virtual IELab. On the horizontal axis are the raw data and on the vertical axis are the violations or deviations of constraint realisations from raw data. The general tendency of the SUT rocket plots on the first row to appear as upward sloping is due to the correspondence of the magnitude of raw data to the magnitude of violation, whereas the pointed shape suggests less variation at the tips for these point constraints.

[15] These standard deviation settings reflect EXIOBASE's philosophy of the primacy of adhering to country SUTs data and preserving the balancing relationships.

The last three rows in Figure 3 show the violations being collected vertically for ratio constraints. Data points located closer to the horizontal axis embody better adherence to raw data. For EXIOBASE2, this improved adherence is most evident for the SUT supply data constraints, as shown by the dominance of light coloured dots associated with EXIOBASE2 below the dark dots of the IELab on the first plot of the first row (Figure 3). For the rest of the row, SUT adherence is shown to improve in the IELab for the final demand and use table components. See the Appendix for a detailed listing of the numerical values of the violations.

These results point to the likelihood that the multiple balancing steps of EXIOBASE2 yield tables with excellent adherence to the balancing constraints but with slightly diminished observance to the various source datasets, as implemented in the IELab. In the original construction method of EXIOBASE2, the trade-linking step introduces an 'international margin layer' as a result of the balancing procedure that inevitably introduces additional deviations between the import data(valued in basic prices in the final multi-region SUT) compared to the original import data with cost, insurance, freight added. This rebalancing essentially controls for the discrepancy between the imports and exports displayed in the country SUT which simply are not balanced at the global level. The IELab procedure apparently allows improvement of adherence to a number of the original data sets (e.g. SUT, AgroSAM), but at the cost of adherence to balancing constraints – which is an important limitation, since MRIOs should, by definition, be fully balanced.

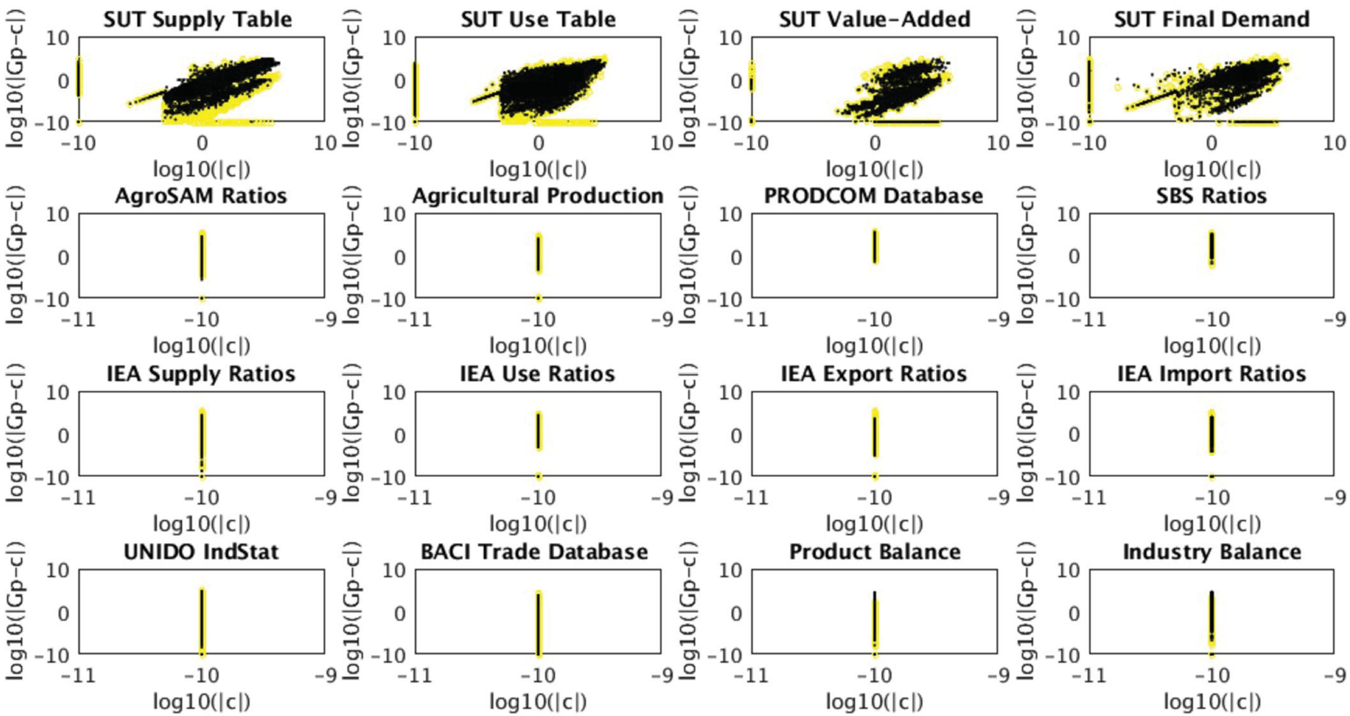
A better understanding of what happens to the data after they undergo processing equips the researchers with useful information for better achieving their aims. In the Lab, the user gains an improved control over several objectives like the degree of desired adherence of the MRIO table to its data sources by assigning varying reliability tags or standard deviation estimates as well as by inclusion or exclusion of constraint sets. On one hand, this flexibility is an advantage but caution must be exercised since this leaves a great deal of discretion to the researcher.

5.2. Case study: EXIOBASE2-based IELab carbon, water, land and material footprints

Since MRIO databases are primarily constructed as research tools capable of providing support to environmental and socio-economic policy decisions, the tables compiled by the IELab are used to calculate global environmental and resource footprints. These IELab results for multiple indicators (carbon, water, land and material footprints) are examined alongside those from the previous comprehensive assessment of Tukker et al. (2014; 2016) based on EXIOBASE data. However, Tukker et al. (2014; 2016) use EXIOBASE version 2.1 in their computation while the IELab uses EXIOBASE version 2.2.3 as its underlying data rendering the direct comparison of the footprints inappropriate. Hence, for consistency, both EXIOBASE2 and the IELab carbon, water, land and material footprints are calculated using EXIOBASE version 2.2.3 data. For both the EXIOBASE2 footprint recalculation and the IELab-based computation, the same per unit of output satellite values, $\mathbf{q}$, are used. In this way, the footprint changes are isolated to reflect the effect of the VL's alternative MRIO construction procedure and specifications.

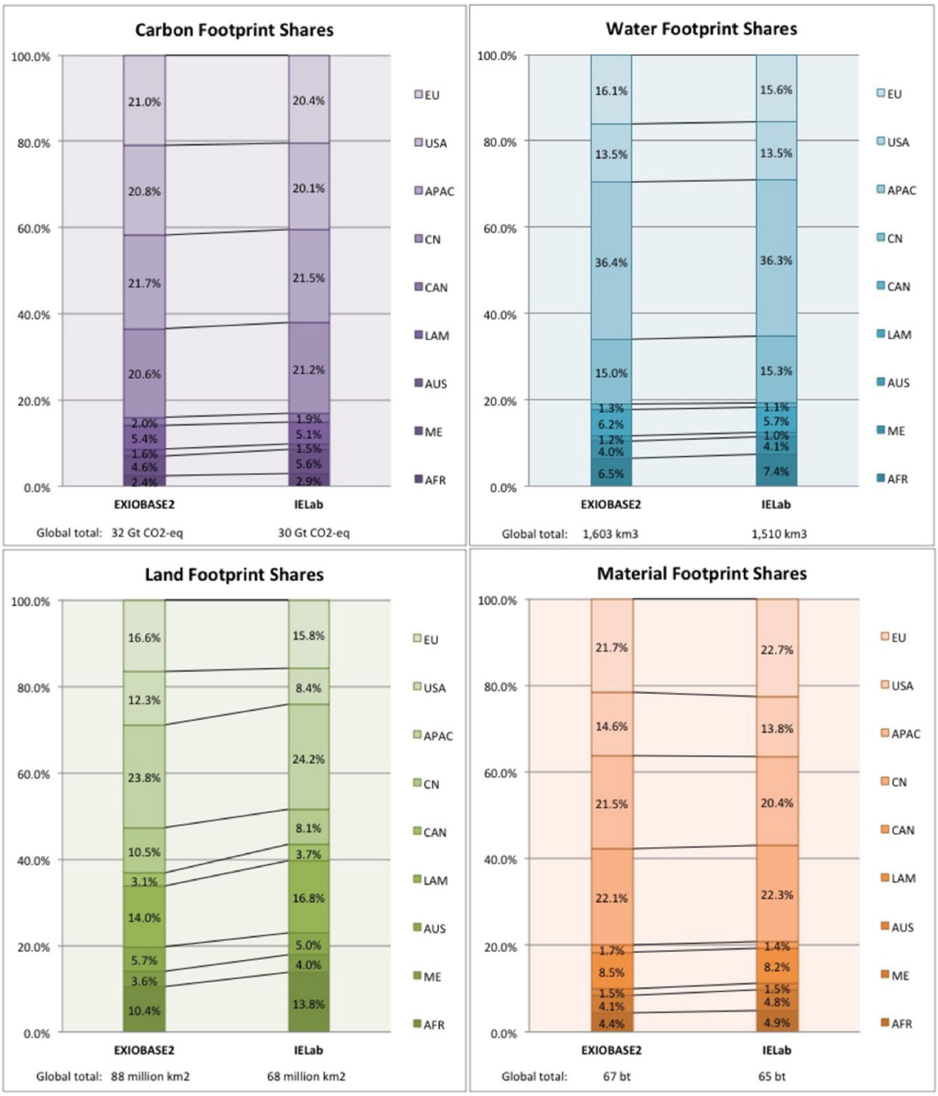
The footprint shares comparison between EXIOBASE2 and the IELab is presented in Figure 4. Note that because IELab has a lower total output and final demand compared

Figure 3. Detailed constraint violations in EXIOBASE2 (light) and IELab (dark), as implemented in the MRIO Lab.



Note: The label on the horizontal axis represents the raw data whereas the vertical axis shows the violations or deviations of constraints realisation from raw data.

Figure 4. Comparison of recalculated EXIOBASE2 and IELab footprints.



Notes: The EXIOBASE2 footprint shares and totals here are for version 2.2.3 and may vary from those reported by Tukker et al. (2014; 2016) calculated with EXIOBASE version 2.1. Abbreviations of regions: EU, Europe; USA, United States of America; APAC, Asia and Pacific; CN, China; CAN, Canada; LAM, Latin America; AUS, Australia; ME, Middle East; AFR, Africa.

to EXIOBASE2, the global totals of all computed footprints are also relatively lower in the IELab.

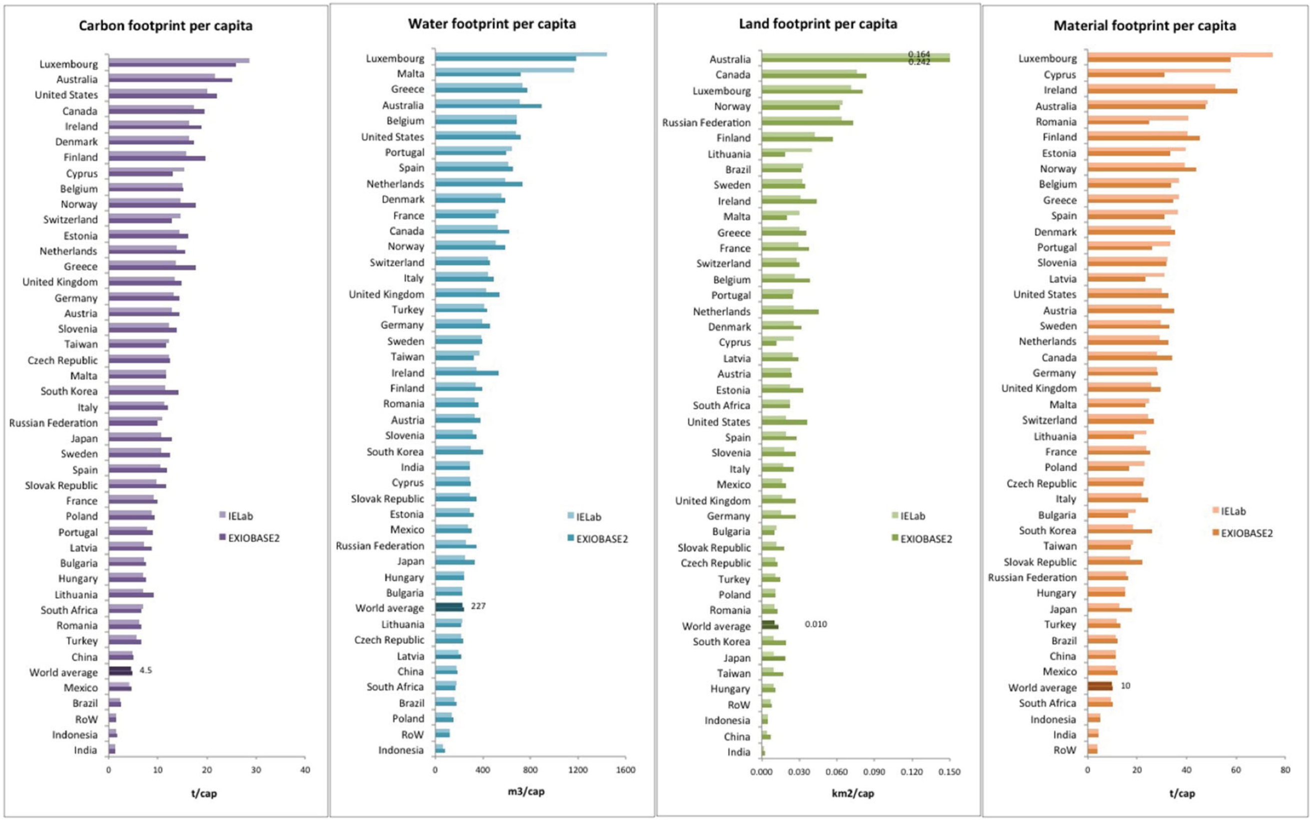
Figure 4 shows that EXIOBASE2 and IELab carbon, water and material footprints are comparable. Across these three indicators, only minimal variation of the footprint shares, if any, is observed for the United States, China, Canada, Latin America and Australia. These regions, collectively, are responsible for 49%, 37% and 47% of the global consumption-based carbon emissions, water and material use, respectively. For the rest of the regions that account for over 50% of the three aforementioned global environmental and resource impacts, there is a slight redistribution of shares arising from the differences between the EXIOBASE2 and IELab MRIOs. Europe's carbon and water footprint shares based on IELab are lower by an average of 0.55%, whereas its material footprint share is 1% compared to EXIOBASE2. Asia and the Pacific region exhibits reduction of carbon, water and material footprint shares from EXIOBASE2 to the IELab while the opposite is the case for the Middle East and Africa. These changes in the distribution of shares and the footprint values may be attributed to the alternate construction procedure in the IELab which alters the resulting Leontief and final demand details. As identified by Owen et al.'s (2014), structural decomposition analysis to explain differences in consumption-based carbon emissions among various MRIO databases, differences in the Leontief inverse and in final demand are among the most significant contributors.

In contrast to the previously discussed indicators, the land footprint shares appear to diverge significantly in Figure 4. This might be a result of large fluctuations of intensities among sectors and their concentration to fewer ones, specifically, the agriculture-related sectors. A further analysis is suggested as a future research avenue in this area to understand what underpins these shifts. One recommended stream of investigation is testing the sensitivity of the land footprints to the AgroSAM and Agricultural Production Output databases ratio constraints. The change in adherence to the ratios provided by these databases may have serious implications on this largely agriculture-related measure. This issue is outside the scope of our study will be explored in future work.

As a general observation, the existence of the variation in footprint information arising from alternative MRIOs serves as a caveat when interpreting indicator estimates since they are associated with some degree of uncertainty and dependent on the philosophy and associated procedures adopted in the MRIO compilation.

Zooming in on country details, per capita footprints are calculated for both EXIOBASE2 and IELab and presented in Figure 5. The figure shows alteration of footprint intensities from EXIOBASE2 to IELab at the national level. The disparities here are expected, as previously reported in Moran and Wood (2014) who highlight discrepancies in carbon footprints of major economies across different MRIO databases, even after harmonising their carbon satellite accounts. EXIOBASE2 and IELab are essentially different databases because of their distinctive compilation processes despite the former being the basis of the latter. Moreover, the change in the IELab balances partly contributes to lower calculated per capita footprints for some countries compared to EXIOBASE. Yet Figure 5 still depicts the uneven distribution of environmental stresses caused by the different regions, as previously reported in Tukker et al. (2014; 2016), with the OECD countries registering well above world average impacts. Luxembourg and Australia consistently appear to have the most intensive environmental effects, partly because of their relatively small population. Additionally, Canada's consumption embodies significant carbon and land use while Ireland's consumption is associated with significant carbon and material footprints. Meanwhile, apart from the lumped rest of the world region, India (with the exception of the water footprint) and Indonesia consistently post the least per capita footprints across the four indicators. South Africa has below average water and material footprints whereas Brazil has below average carbon and water footprints. These findings support the well-established fact that developing countries have smaller consumption-based per capita impacts.

Figure 5. Recalculated EXIOBASE2 and IELab footprints per capita.



Note: The EXIOBASE2 footprints per capita here are for version 2.2.3 and may vary from those reported by Tukker et al. (2014; 2016) calculated with EXIOBASE version 2.1.

6. Conclusions and outlook

Within the umbrella project of the Global MRIO Virtual Laboratory, this work serves as a proof of concept on how one of the major world MRIO databases, EXIOBASE2, can be implemented into a Virtual Laboratory context. The construction of the original EXIOBASE2 database employs a multiple balancing procedure that comprises balancing of country SUTs at the detailing/harmonising step and balancing of the whole database at the conclusion of the trade-linking step. The IELab offers a shortcut to this procedure by not replicating the full EXIOBASE2 production process. Instead, the already detailed final version of the EXIOBASE2 database is used as the starting point ('initial estimate'). This strategy allows the IELab workflow to forego the first, complex and labour-intensive detailing and balancing step at the country level performed in the construction of the original EXIOBASE2 database. While in the EXIOBASE2 procedure the final balancing involves using only the trade data, the setting of the IELab allows the use of a variety of other source data, even those that are conflicting, as constraints in the one-time balancing. The ideal construction of the Lab version of EXIOBASE2 entails defining the IE from raw and not pre-processed data. However, this requires more time and resources beyond the scope of the current project.

An important feature acquired through bringing EXIOBASE2 to the Lab setting is flexibility. Any EXIOBASE2-based table, within the limits of its root classification, may be generated in a highly automated approach. In a less intensive user-input process, the researcher can exercise control over various objectives. The researchers gain influence over the choice of relevant constraint sets and the MRIO table's degree of adherence to various data sources relevant to their research questions. For instance, flexibility in the level of degree of adherence to IEA constraints (for energy-focused research) or AgroSAM constraints (for agriculture-related studies), or supplementing EXIOBASE with new superior dataset, becomes possible.

The IELab table presented in this paper is compiled according to the original EXIOBASE2 philosophy of the primacy of preserving SUT information and building a well-balanced table. Interestingly, the diagnostics applied to this IELab table reveal its stronger adherence to all source data but a less balanced table compared to the original EXIOBASE2 database. A major implication drawn is that where the original EXIOBASE2 construction procedure leads to almost perfect adherence to balancing constraints, the condensed IELab approach, that reconciles the MRIO elements to many conflicting source data while balancing, shifts the priority away from balancing, resulting to a compilation of a less balanced table. This is a drawback whenever fully balanced tables are required (e.g. in CGE models).

For illustration of MRIO-based calculation, footprints of carbon dioxide-equivalent (CO2-eq) global warming potential (GWP), blue water consumption (surface and ground water withdrawals), land use and raw material consumption (RMC) are calculated using an IELab table derived from the EXIOBASE2 data and compared with EXIOBASE2's footprints and footprint shares viewed at a macro level. Since the IELab table used is less balanced than the original, the change in the balances results to lower environmental and resource impacts, overall. With the exception of land, the distribution of environmental footprints in the IELab remains unchanged for many regions but varies slightly for the regions responsible for more than half of the global impacts. For land, further analysis is suggested as future work to unveil the driver of the large divergence in regional footprint shares. The foregoing points to the sensitivity of such indicators to the approach adopted in building the MRIO tables. Thus, a recommended stream of investigation on the land footprints is towards testing their sensitivity to the AgroSAM and Agricultural Production Output databases ratio constraints. The change in adherence to the ratios provided by these databases may have serious implications on this largely agriculture-related measure. Additionally, the IELab per capita footprints highlight the expected inequality of environmental stresses caused by developed and developing countries, with the citizens of the former being responsible for greater impacts.

The initial steps taken in this work on bringing EXIOBASE to a common platform with other prominent MRIO databases pave the way for combining the best features of various MRIO databases in the future. This presents new opportunities for further improving global MRIO compilation in terms of process and quality, consequently, making the outcome of MRIO-based analyses more relevant on informing environmental and socio-economic policy decisions.

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