

Matrix-based Methods for Regionalized Life Cycle Assessment

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Abstract

We develop a comprehensive computational framework for matrix-based regionalized life cycle assessment (LCA). When life cycle inventories and impact assessment methods have different spatial scales, spatial allocation is needed to map inventory locations to impact assessment spatial units. We review spatial allocation based on intersected areas and existing background emissions, and propose using additional spatial inventory data as a third type of allocation, which we call extension tables. Extension tables allow for detailed maps of individual processes, or even separate maps for specific process emissions — a significant improvement over the assumed uniform spatial density of process datasets. Extension tables can also be applied to existing process datasets. New LCA matrix formulae are developed for all three forms of spatial allocation, and these formulae allow for the expression of results on multiple spatial scales. As the final calculation result is a matrix, instead of a single value, the most damaging processes, emissions, and spatial units for every spatial scale used can be easily identified and combined. A case study of ecosystem damage due to freshwater consumption from irrigation of cotton in the United States is used to illustrate the different approaches. We implement our framework in an accessible open-source software package, including multiple additional examples.

Introduction

Life cycle assessment (LCA) is a technique to calculate the life cycle environmental impacts of goods and services. LCA distinguishes between life cycle inventories, which describe each step of a technological supply chain, including final disposal; the emissions and resource consumption accompanying each step; and life cycle impact assessment (LCIA), which characterizes the damage done by the emissions and resource consumption.

The importance of including spatial variation in both technological processes and the natural world has been recognized since the development of LCA in the 1990s.¹ LCA studies that are *site-generic* – those which do not include any differences in production technologies or environmental sensitivities around the globe – are limited in the types of decisions that can be supported. LCA studies that are *site-specific* – whose conclusions are specific to a certain plant location or receiving environment, such as obtained from environmental impact assessment – cannot be scaled up to provide a comprehensive global picture of technological production and environmental impact. The inclusion of spatial variation is therefore called “regionalization”, as regions, which can range from tens to thousands of square kilometers, are a natural spatial scale for performant and comprehensive LCA calculations.¹

For inventory data, regionalization means a detailed description of the location where an inventory dataset occurs, preferably including spatial coordinates. Regionalized inventory datasets are most accurate when their spatial locations are as parsimonious and representative as possible. For example, a dataset for cotton cultivation in the USA should not include Alaska, and ideally would be limited to the states or counties where cultivation actually occurs. Some inventory data formats allow locations to be described with spatial coordinates, while others are limited to a name or the latitude and longitude of a single point.^{2,3}

A number of regionalized impact assessment methods with a global scope have been recently developed, including impact categories such as land and water use, ecosystem services, and air and water emissions.⁴⁻¹⁸ There is no standard data format for supplying characterization factors from regionalized impact assessment methods, nor do most method developers provide a justification for the chosen impact assessment spatial scale. Despite these limitations, the

production of many regionalized impact assessment methods is a significant step towards more accurate characterization of environmental impacts in LCA.

Several techniques for performing regionalized LCA have been described in the literature. Early studies manually matched regionalized characterization factors to inventory locations, though this approach has not been formally specified.^{19,20} Such manual matching can be done for foreground processes – the first few steps in the direct supply chain of the examined good or service – but is not feasible for the thousands of inventory datasets which make up the background model of the industrial economy used in LCA. Manual matching also requires that inventory datasets and LCIA methods share the same spatial scale.

Another approach is to use two separate models: a site-generic LCA model for background processes, and a separate geographic information system (GIS) model for regionalized foreground calculations.²¹ This approach can include more detail, and can be more complex than normal LCA models, as it can include nonlinearities and feedback effects. However, this complexity is also a drawback, for most LCA practitioners do not have the time or expertise to develop GIS models for each LCA study. Data transfer between the two models has also been difficult.

The use of raster datasets has also been proposed for regionalized LCA. One could treat each raster cell as a separate activity, though it is difficult to imagine how such an approach could scale beyond simple case studies.²² Raster maps probably have more potential as external data sources that can be combined with inventory results. Feeding raster maps of activity parameters into LCIA models could offer significant advantages, especially if multiple environmental stressors could be assessed simultaneously.²³ Combining rasters with different spatial scales requires spatial interpolation, and there is not yet a general approach for including raster maps describing different aspects of individual activities which is applicable to an entire LCA calculation.

The standard calculation methodology of LCA can also be adapted to include regionalization. Nansai and colleagues showed how to construct matrices with region-specific characterization factors, assuming that the inventory and impact assessment method shared the same spatial scale, but for only one environmental flow at a time.²⁴ We earlier developed a matching algorithm to create region-specific characterization factor matrices for all environmental flows, again assuming a shared spatial scale.²⁵ We also described how a mapping matrix can be used to allocate inventory datasets with spatially uncertain point geometries to impact assessment locations.²⁶ Yang and Heijungs developed a general matrix structure for regionalized LCA with a shared spatial scale.²⁷ None of these approaches, however, provide a complete framework for the spatial allocation of inventory datasets to multiple impact assessment locations.

In this paper, we develop a comprehensive calculation framework for regionalized life cycle assessment. We show how to spatially allocate inventory datasets to multiple impact assessment locations based solely on intersected area, or by using additional background inventory or impact assessment data. We also show how to combine these different approaches, and how to interpret regionalized LCA results on multiple spatial scales. A case study of cotton production in the USA is used to demonstrate the framework.

Methods

Symbology

Table 1: Symbols, vectors, and matrices used in this manuscript, along with their dimensions and explanations.

Symbol	Dimension(s)	Explanation
e		A single elementary flow, e.g. carbon dioxide.

p		A single inventory dataset, e.g. making 1 kg of steel.
i		A single inventory spatial unit, e.g. Canada.
j		A single impact assessment spatial unit, e.g. the Rhine watershed.
z		A single extension table spatial unit, e.g. a raster pixel.
E	e	The set of elementary flows, $e \in E$.
P	p	The set of inventory datasets, $p \in P$.
I	i	The set of inventory spatial units, and i is a single inventory spatial unit, $i \in I$.
J	j	The set of impact assessment spatial units, $j \in J$.
Z	z	The set of extension table spatial units, $z \in Z$.
A	P,P	Technosphere matrix that specifies the amount of each inventory dataset input needed for each inventory dataset output.
B	E,P	Biosphere matrix that provides elementary flow values associated with each inventory dataset.
C	E,E	Diagonal characterization matrix that gives characterization factors for each elementary flow.
f	P	Demand vector that defines the functional unit being analyzed, i.e. the amount of each inventory dataset output.
h	E,P	Characterized inventory matrix that gives the impact associated with each elementary flow and inventory dataset output needed for the functional unit. The sum of all elements in h is the total LCA score.
M	P,I	Mapping matrix that maps inventory datasets to inventory spatial units. If an inventory dataset p occurs in inventory spatial unit i , $\mathbf{M}_{p,i} = 1$; otherwise, it is zero.
R	J,E	Regionalized characterization matrix that gives characterization factors specific to each elementary flow and impact assessment spatial unit.
G	I,J	Geographic transform matrix that provides the area of impact assessment spatial unit j in each inventory spatial unit i , $\mathbf{G}_{i,j} = \text{area}(i \cap j)$.

L	J,J	Diagonal background loading matrix that indicates the emissions density in each impact assessment spatial unit.
D	I,Z	Distribution matrix that provides the area of inventory spatial unit i in each extension table spatial unit z , $\mathbf{D}_{i,z} = area(i \cap z)$.
X	Z,Z	Diagonal extension table matrix that indicates the extension table density value in each extension table spatial unit.
N_G	I,I	Diagonal normalization matrix.
N_{GL}	I,I	Diagonal normalization matrix.
N_{DX}	I,I	Diagonal normalization matrix.

We start by defining some common symbols that will be used throughout this manuscript in Table 1. Elementary flows are the objects in LCA for which a damage or benefit is assessed, and can include physical flows, such as emissions to air, soil, or water, and consumption of resources. They can also include social and economic flows, as often reported in input-output analysis. Inventory datasets describe an activity that consumes inputs and produces one or more outputs. Spatial units are sets of data about a location, including its spatial support (the actual coordinates that define its boundaries in a given coordinate reference system), as well as its name, abbreviation, and other metadata.

Three types of spatial allocation

Spatial allocation is known in the geographic literature as a change of spatial support;²⁸ in regionalized LCA, spatial allocation is used to allocate inventory processes to impact assessment spatial units, in order to apply the correct characterization factors. The idea of a spatial allocation matrix is to distribute processes and their respective emissions without changing the emission totals, and therefore each row in a spatial allocation matrix should normally sum to one, and each value in that matrix should be between zero and one. In some special cases, when an inventory location does not intersect any impact assessment spatial units, a row may sum to zero. In this case,

one can either leave the row sum of zero, meaning that this process would have no characterization factors applied, and hence no calculated impact, or apply global average characterization factors. Both options are considered in the discussion section “Inventory locations outside impact assessment maps.”

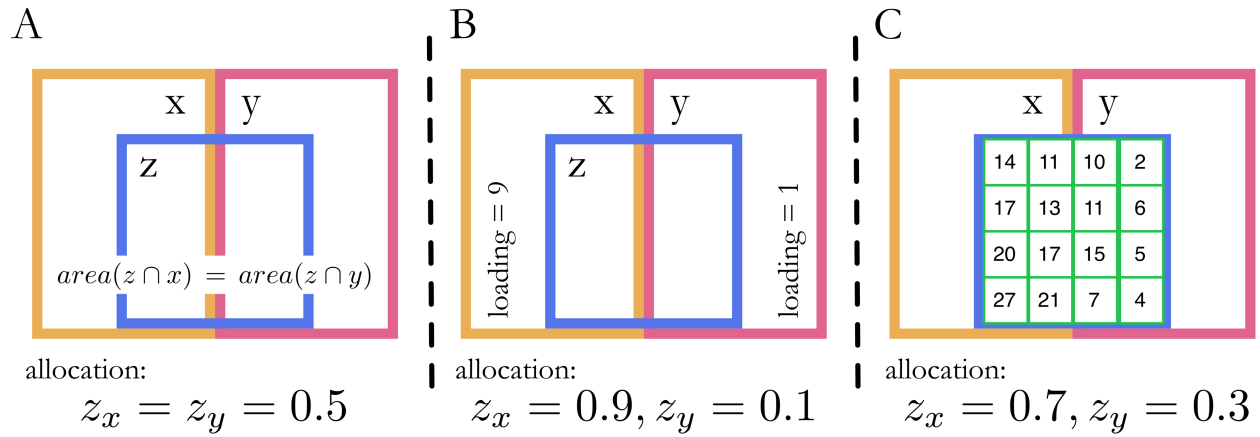


Figure 1. Three approaches for the spatial allocation of inventory unit z to impact assessment units x and y . *A* shows allocation based on intersected area. In this case, z is equally split between x and y , so the allocation is 0.5 for each. *B* shows allocation based on background emission loadings, and there are significantly more emissions in x than y , leading to x having a higher allocation factor. *C* shows allocation based on additional detailed spatial inventory data. In this case, the sum of the detailed inventory values in x is higher than in y , so x again has a higher allocation factor.

Table 2: Formulae for three spatial allocation matrices.

Spatial Allocation Type	Formula
Areal intersections	$\mathbf{N}_G \mathbf{G}$
Background loading (additional data on impact assessment scale)	$\mathbf{N}_{GL} \mathbf{GL}$
Extension tables (additional data on a new spatial scale)	$\mathbf{N}_{DX} \mathbf{DX}$

We describe three types of spatial allocation, shown in Figure 1A-C, and defined in Table 2. First, in the absence of additional data, allocation of inventory locations to impact assessment spatial units can be done based on their respective intersected areas. Figure 1A shows that inventory location z would be equally allocated to impact assessment locations x and y , as its area is equally split between the two.

Figure 1B shows spatial allocation based on background emissions loadings. By the term background loadings, we mean the current emissions and resource consumption due to status quo economic activities. In our conception, background loading values are provided by the impact assessment method developers, as most impact assessment methods provide marginal characterization factors, whose calculation usually includes knowledge of the spatial pattern of existing emissions.²⁹ We acknowledge that background loadings are imperfect predictors of the spatial pattern of *sources*, as the inputs to impact assessment methods are the background concentrations, which represent flow *sinks* after transport. Background loadings can be provided on the impact assessment spatial scale, and their values function as weights, as in a weighted average, but we avoid the term weighting as it already has a specific meaning in impact assessment.

Finally, Figure 1C shows spatial allocation based on additional spatial inventory data. Existing matrix-based LCA calculation methodologies assume that each inventory dataset has one location, with uniform areal density. This assumption is usually made due to a combination of limited data availability and a lack of suitable data formats for storing such disaggregated inventory data. For example, previous version of the US LCI has a single inventory dataset for “Cotton, whole plant, at field” for the entire USA,³⁰ though more detailed information from other sources is available for e.g. irrigation water consumption³¹ and fertilizer application amounts.³² This additional spatial inventory data has its own spatial scale, one not linked to the spatial scale of the inventory

processes. This detailed background data can be used to describe the spatial pattern of inventory processes.

Additional inventory spatial data does not fit into existing inventory data formats but does fit well into a spreadsheet with columns of inventory spatial unit, extension table spatial units, and one or more data columns; we therefore call these additional data extension tables.

Each spatial allocation matrix in Table 2 includes a normalization matrix. Normalization matrices are used to ensure that a given row or column sums to one. For example, in equation 1, the normalization matrix transforms from the absolute intersected area of spatial units i and j to the intersected area of i and j relative to the total area of i intersected by all spatial units in J . These matrices are defined in equations 1, 2, and 3 below. For all three normalization matrices, if the equation gives an undefined value (i.e. division by zero), a value of zero is inserted.

$$\mathbf{N}_{G_{i,i}} = \left(\sum_{j \in J} \mathbf{G}_{i,j} \right)^{-1} \quad (1)$$

$$\mathbf{N}_{GL_{i,i}} = \left(\sum_{j \in J} [\mathbf{GL}]_{i,j} \right)^{-1} \quad (2)$$

$$\mathbf{N}_{DX_{i,i}} = \left(\sum_{z \in Z} [\mathbf{DX}]_{i,z} \right)^{-1} \quad (3)$$

Background loadings and extension table values (matrices \mathbf{L} and \mathbf{X}) need to be given as flows per unit area. Using absolute amounts would produce biased answers in cases where the spatial units J and Z had heterogeneous sizes or were incompletely covered by other spatial scales. A graphical example of this bias is shown in the supporting information (SI).

Calculation methodologies for regionalized LCA

Table 3: Matrix calculation methodologies for site-generic and regionalized LCA. “ \circ ” is the symbol for the Hadamard product, also known as the entrywise or elementwise product.³³

Result Dimensions	Formula
0: Site-generic	

E,P	$\mathbf{CB} \cdot \text{diag}(\mathbf{A}^{-1}f)$
1: Shared Spatial Scale	
E,P	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)] \circ [\mathbf{MR}]^T$
E,I	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)]\mathbf{M} \circ \mathbf{R}^T$
2: Two Spatial Scales, Areal Allocation	
E,P	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)] \circ [\mathbf{MN}_G\mathbf{GR}]^T$
E,I	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)]\mathbf{M} \circ [\mathbf{N}_G\mathbf{GR}]^T$
E,J	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)]\mathbf{MN}_G\mathbf{G} \circ \mathbf{R}^T$
3: Two Spatial Scales, Background Loading Allocation	
E,P	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)] \circ [\mathbf{MN}_{GL}\mathbf{GLR}]^T$
E,I	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)]\mathbf{M} \circ [\mathbf{N}_{GL}\mathbf{GLR}]^T$
E,J	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)]\mathbf{MN}_{GL}\mathbf{GL} \circ \mathbf{R}^T$
4: Two Spatial Scales, Inventory Extension Tables	
E,P	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)] \circ [\mathbf{MN}_{DX}\mathbf{DXN}_G\mathbf{GR}]^T$
E,I	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)]\mathbf{M} \circ [\mathbf{N}_{DX}\mathbf{DXN}_G\mathbf{GR}]^T$
E,J	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)]\mathbf{MN}_{DX}\mathbf{DX} \circ [\mathbf{N}_G\mathbf{GR}]^T$
E,Z	$[\mathbf{B} \cdot \text{diag}(\mathbf{A}^{-1}f)]\mathbf{MN}_{DX}\mathbf{DXN}_G\mathbf{G} \circ \mathbf{R}^T$

Table 3 gives calculation formulae for five calculation methodologies, from site-generic to regionalized LCA. As the level of spatial detail increases, the number of ways the final result can be expressed increases as well; for method four, the result matrix can be calculated with dimensions of elementary flows by inventory processes, or by inventory spatial units, or by impact assessment spatial units, or even by extension table spatial units.

Note that we do not use the term $(\mathbf{I} - \mathbf{A})$, which assumes that each process produces only one unit of output, an assumption that does not hold in modern inventory databases;² rather, our \mathbf{A} matrix includes both inputs (negative values) and outputs (positive values).

Method 0: Site-generic LCA

Method 0 is the standard formula for matrix-based LCA.³⁴ This formula is site-generic – there is no spatial differentiation of impact assessment characterization factors, and inventory dataset locations are not specified. It will, however, serve as the foundation on which regionalized data and matrices can be added.

Method 1: Shared spatial scale

If the impact assessment method is regionalized, and if the inventory and impact assessment spatial scales are the same, then method 0 can be modified to provide characterization factors specific to each inventory dataset location. Method 1 shows how the site-generic characterization matrix \mathbf{C} is replaced by the \mathbf{M} and \mathbf{R} matrices.

We earlier developed a different version of method 1, where \mathbf{M} and \mathbf{R} were multiplied to give the matrix \mathbf{R}' , with dimensions P, E .²⁵ We prefer the formulation given in table 3, as it avoids the need in \mathbf{R}' to repeat characterization factors for each instance of the same inventory spatial unit, and provides the foundation for additional methods.

Method 2: Different spatial scales with areal allocation

When the inventory database and impact assessment method have different spatial scales, but no background loading is available, calculations can be made using method 2. We earlier derived a slightly different form of method 2, which combined the \mathbf{N}_G and \mathbf{R} matrices.²⁶ We prefer the form given here, as it clearly separates the normalization and characterization steps.

Method 3: Spatial allocation using background emission loadings

When the inventory database and impact assessment method have different spatial scales and emission or resource-use loadings are available (on scale J), calculations can be made using method 3.

Method 4: Spatial allocation using inventory extension tables

When the inventory database and impact assessment method have different spatial scales and additional spatial inventory data is available, calculations can be made using method 4. As this method matches three different spatial scales (extension tables, inventory, and impact assessment), two spatial allocation steps are necessary.

Combining methods

Calculation methodologies can be combined when different levels of detail are available for different selected datasets. To use a different methodology for a few datasets, do a general calculation for the rest of the system, but remove the selected datasets from the **M** matrix. A separate calculation, potentially using a different calculation methodology, can then be done using an **M** matrix that maps only the selected datasets. The total result will simply be both calculations added together. Background datasets could also be split into broad categories, so that separate background loadings could be used for method 3. For example, the spatial pattern of nitrogen emissions from transportation processes is different than that of agricultural processes. For method 3 and 4, different spatial patterns can even be provided on a biosphere flow-specific level, by using multiple **R** matrices, each containing characterization factors for only the selected biosphere flows. The additivity of the different methods gives the ability to calculate detailed results using the best data for each inventory dataset and biosphere flow, with the only restriction being that all processes and flows are accounted for in at least one calculation type.

Interpretation of regionalized calculations

When the result matrix has dimensions E,P , it has exactly the same form as the standard characterized inventory matrix **h**. The largest entries of this matrix show the most damaging combinations of elementary flows and activities. Summing the rows (elementary flows) of this

matrix gives the most damaging inventory datasets, and summing the columns (inventory datasets) gives the most damaging elementary flows.

In addition to calculating \mathbf{h} , we can also interpret the results on different spatial scales. Depending on the result matrix dimensions, summing the rows can give the most damaging inventory, impact assessment, or extension table spatial units.

Implementation in open-source software

The calculation methodologies are implemented in *brightway2-regional*, an open-source LCA software package. *brightway2-regional* includes several implementation optimizations, including faster calculations of extension table matrices and the use of topographical mappings to only calculate intersections of the same regional borders once. \mathbf{G} matrix areal intersection calculations were made using *pandarus*, a separate open-source software utility³⁵. In addition to the source code, the SI gives links to extensive online documentation for both pieces of software.

Case study of irrigated cotton

We conduct a case study of cotton production in the USA to illustrate the different computational methods. The impact assessment method used is ecosystem damage from surface water consumption, for which characterization factors are available with multiple spatial scales: 0.5 degree raster grids, US states, and countries.⁴ The unit for this impact assessment method is potentially disappeared fraction (PDF) of species per square meter per year. Inventory data on irrigation from surface waters came from the USDA LCA commons database, version 1.1^{36,37} and production totals came from NASS;³² both are available for individual states. County-level background loading data on surface water use came from USGS³⁸. All data preparation and calculations are documented in the online scientific notebooks included in the SI.

Results

Table 4 shows case study LCA scores for the five calculation methodologies, using a functional unit of one kilogram of the national production mix of cotton lint. The electronic SI also shows results for corn, soybeans, and winter wheat. In this case study, method zero uses an average characterization for the USA, which includes many areas without significant stress, and it is no surprise that the score is therefore low compared to the other methodologies. In method one, both impact assessment and inventory share the spatial scale of states within the USA. State-average characterization factors are more specific than one national average factor, but will still average over entire states, including areas of water abundance and scarcity. For example, the state average characterization factor for California combines the water availability in the North with the scarcity in the South. The total LCA score for method 1 is therefore higher than method 0, but less than the other methods.

Table 4. LCA scores in $\text{PDF}\cdot\text{m}^2/\text{year}$ for one kilogram of the national production mix of cotton lint for one site-generic and four regionalized calculation methodologies.

Calculation Method	LCA score ($\text{PDF}\cdot\text{m}^2/\text{year}$)
0: Site-generic	0.255
1: Shared spatial scale	0.886
2: Two spatial scales	1.39
3: Two spatial scales with loading	2.38
4: Inventory extension tables	2.21

The different scores for methods 2, 3, and 4 reflect the data used to calculate the spatial allocation of inventories to impact assessment spatial units. Method 2 uses the intersected areas of states and watersheds; method 3 uses values on total irrigation within each watershed; and method 4 uses

detailed model data on irrigation of cotton. The difference in score between Method 3 and Method 4 reflects the difference between the relative impact of spatial pattern of all irrigation in each state versus the specific spatial pattern of cotton production. Cotton and other irrigated crops appear to be grown in (and are perhaps contributors to) areas of high water stress. Figure 2 shows the spatial pattern of ecosystem damage from irrigation freshwater consumption for methods 3 and 4.

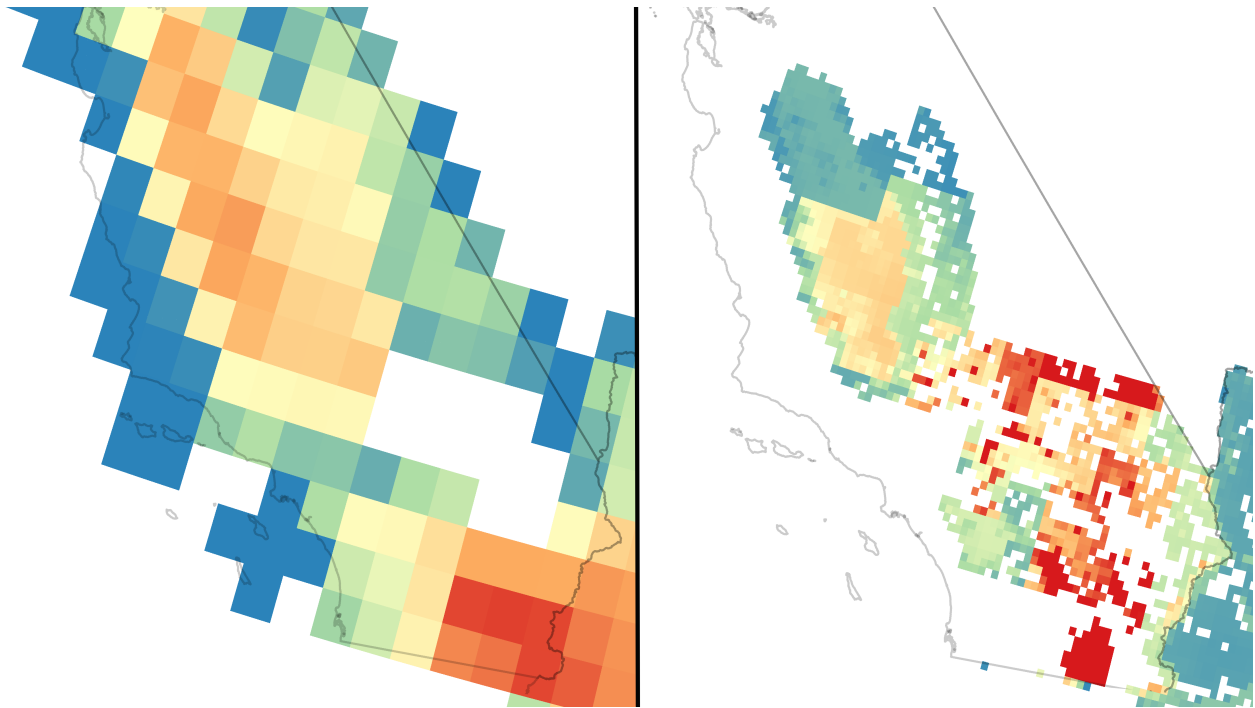


Figure 2. Comparison of the spatial pattern of environmental impact in southern California using methods 3 (Two spatial scales with background loading) and 4 (Two spatial scales with inventory extension tables). Impact was calculated for ecosystem impact due to the consumption of surface water for irrigated production of cotton lint. Impact is mapped to a color scale, from low (blue) to high (red). Because of the differing spatial resolutions, a common color scale would be deceptive. The large white hole for method 3 is a result of San Bernardino county reporting zero water irrigation surface-water withdrawals.

Discussion

Calculation methodologies

Encapsulating regionalized LCA in matrix equations brings a number of advantages. Matrix math is fast, precise, and easy to understand. Matrices also allow for the efficient application of uncertainty and sensitivity analysis. Finally, matrices allow regionalized LCA results to be easily expressed in multiple spatial scales.

As more regionalized inventory databases and impact assessment methods become available, regionalized LCA should produce more accurate results, and therefore should be preferred to site-generic assessments. However, no single method of spatial allocation is strictly better than any other. In general, the use of higher resolution data should produce more accurate results. The choice of allocation method, however, should reflect the tradeoff between the expected gain in result accuracy from more detailed methods versus the opportunity cost of increasing data quality elsewhere in the LCA model. One possibility for a systematic approach is to start with less detailed data, and selectively increase data resolution and quality based on sensitivity analysis.³⁹

Extension tables also allow multiple inventory spatial patterns to be used for different biosphere flows from the same inventory process. At first, this may seem strange, as an inventory process dataset is defined with a uniform density for one product system in one place and time. However, in practice process datasets often aggregate groups that have different characteristics, such as older and newer coal-fired power plants, or agricultural crops that are grown both extensively and intensively in a given country. Extension tables can also be used to split aggregated process datasets or industry sectors, such as splitting “vegetables” into cucumbers, onions, etc.⁴⁰

With additional methodological development, calculation methods based on raster algebra could be an attractive alternative to the vector-based methods given in this paper. In theory, the use of raster maps could be fast, memory-efficient, and produce detailed results. In the context of LCA,

a comprehensive method would need procedures for uncertainty propagation, characterizing uncertainty from interpolation, and guidance on data and metadata formats. Of particular interest would be the delegation of site-specific impact calculations to external models which could include multiple environmental stressors – a technique we have previously labelled “offshoring”. We note that such activity-specific offshored results can be easily included in our methodology.

Case study results

The case study is intended only to show the different calculation methods applied to real-world data. It is limited by the available inventory data, and does not examine other areas of protection, such as human health, or include irrigation from groundwater and its consequences. Its conclusions are therefore not indicative of total environmental performance. The accuracy of the damage from surface water consumption results could be improved with the use of more detailed inventory data, such as county- instead of state-level spatial units, and with higher temporal resolution, such as monthly instead of yearly water withdrawal values and characterization factors.³¹

In general, each increase in the spatial complexity of the calculation methodology, i.e. from method one to method two, or from method two to method three, led to a higher LCA score. This is consistent with impacts from water consumption being driven primarily by freshwater scarcity due to irrigation. Background loadings give a higher weight to areas where there is already substantial irrigation, and the existing irrigation increases water stress and therefore increases characterization factors. Decreasing the level of spatial detail causes averaging effects to reduce the total score. However, this pattern would not be true for other environmental flows such as land use. The relationship between regionalized and site-generic results will depend on the correlation between the spatial patterns of inventory datasets, background loadings, and characterization factors.

Inventory locations outside impact assessment maps

If an impact assessment method does not provide complete global coverage, then it is possible that some inventory spatial units or parts of inventory spatial units may lie outside any impact assessment spatial units. In the extreme case, an entire inventory spatial unit could be outside any impact assessment spatial units. Examples include offshore processes omitted by land-based impact assessment methods, and impact assessment methods with limited spatial coverage used with an assessment of global supply chains. There are two approaches for handling such inventory spatial units.

The easy approach is simply to ignore these unintersected areas, so that the sections of the inventory spatial unit that do intersect impact assessment spatial units will determine the regionalized result. The alternative is to apply a global average characterization factor in such cases. Both approaches can be used in calculation methodologies 1 to 4, although we note that the common practice of adding a “global” inventory location to the set of inventory spatial units is required.

Depending on the functional unit and impact assessment method, either approach could be more appropriate. Ideally, method developers will provide explicit guidance on when and which global characterization factors should be applied. In the meantime, both approaches should be tried as a simple sensitivity test. A large difference in LCA scores for the two methods is an indication that the chosen impact assessment method is not recommended for the system being studied. Software could also implement a user warning when, for example, more than 10 percent of an inventory’s area would be excluded. Additional studies could help examine this issue more thoroughly.

To avoid this dilemma, we strongly encourage LCIA method developers to recognize the difference between null, where no characterization factor is provided, and zero, where there is no

calculated damage from an environmental flow. Characterization factors with a value of zero should be included wherever appropriate.

Outlook

In the **G** matrix, we assume that most inventory spatial units will be polygons or multipolygons. Points and linestrings with spatial uncertainty can be treated as polygons, as shown in earlier work.²⁶ Linestrings without spatial uncertainty can be allocated based on their respective intersected lengths, and points with spatial uncertainty can be allocated equally to each impact assessment spatial unit they intersect.

Instead of using process- or industry-specific background loadings, some have proposed using population density as a generic proxy for industry spatial activity. This is a promising approach that avoids new data collection, and may be especially useful for calculating aggregated, site-generic characterization factors. The use of population density as a proxy for the spatial patterns of specific industries should be justified, however, given the mixed messages of existing literature.⁴¹ While industrial facilities may be good predictors of population centers, not every population center will have industrial facilities from each industry sector.

Regionalization can increase the power and accuracy of LCA calculations. We developed calculation methodologies for regionalized LCA covering three types of spatial allocation from inventory to impact assessment spatial units. Areal allocation is simple to understand and calculate but can produce misleading results. Many impact assessment methods calculate marginal characterization factors, which require a database of background emission loads. These background emission loading values can be used to estimate existing spatial patterns of industrial activity. Finally, additional inventory data can be used to disaggregate process datasets or even provide spatial pattern maps for individual biosphere flows. This additional inventory data can be expressed as a series of extension tables that supplement existing inventory data formats, which

assume uniform spatial density. In addition to identifying the most damaging processes and biosphere flows, LCA calculation results can be transformed to the inventory, impact assessment, and extension table spatial scale. We provide an open-source implementation of our work as an add-on for the Brightway calculation framework.⁴²

Supporting Information

The supporting information includes online scientific notebooks describing all case study data preparation and calculations, and additional case study figures. The software *pandarus* and *brightway2-regional* are also described, and links are given to their source code and documentation, as well as other examples of regionalized calculations using our software.

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The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript.

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Supporting Information for “Matrix-based Methods for Regionalized Life Cycle Assessment”

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Open-source software

Brightway2-regional

Brightway2-regional is built on top of the [Brightway2 LCA software framework](#). As such, it provides the functionality related to storing, processing, and calculating regionalized inventories, impact assessment methods, and LCA results.

Brightway2 and *Brightway2-regional* are written in Python, and use common Python scientific packages such as *scipy* and *numpy*, and common python geospatial packages like *rasterio*, *shapely*, and *fiona*. All of *Brightway2* is 3-clause BSD licensed.

The online documentation and manual is available here: <http://brightway2-regional.readthedocs.org/>

The source code is available here: <https://bitbucket.org/cmutel/brightway2-regional>

Pandarus

Pandarus is a utility for matching two geospatial datasets, and calculating the intersected areas of each pair of intersecting spatial units. Its output can be directly imported into *Brightway2-regional* to construct the geographic transform matrix **G**.

The online documentation is available here: <http://pandarus.readthedocs.org/>

The source code is available here: <https://github.com/cmutel/pandarus>

Other compatible open-source software

Pandarus-remote

pandarus_remote is a web service for processing and managing data for regionalized life cycle assessment using *pandarus*.

Source code: https://github.com/cmutel/pandarus_remote

Rower

Consistently define, label, and manage "Rest-of-World" locations for processes in Brightway databases. ecoinvent Rest-of-Worlds definitions: <https://geography.ecoinvent.org/rows/>

Source code: <https://github.com/PascalLesage/Rower>

Brightway2-LCIMPACT

This package provides the impact of the [LC IMPACT](#) regionalized LCIA method in *brightway2* and *brightway2-regional*.

Source code: <https://github.com/cmutel/bw2-lcimpact>

Constructive geometries

Simple tools to define world locations from a set of topological faces and set algebra. For example, one could define a "rest of the world" which started from all countries, but excluded every country whose name started with the letter "a".

Documentation: <https://constructive-geometries.readthedocs.io/>

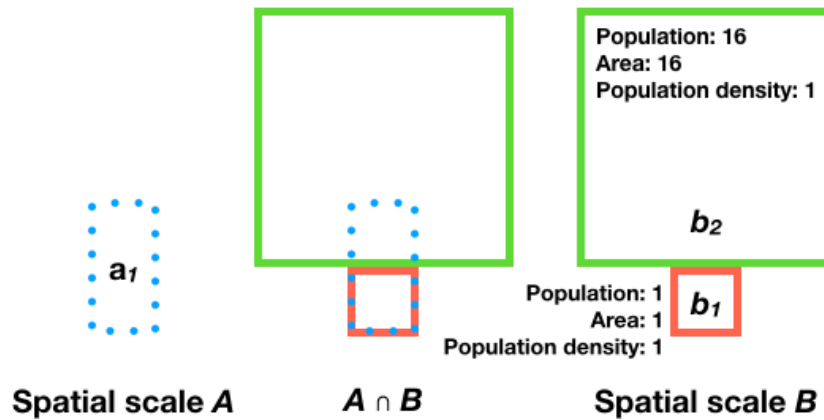
Source code: https://github.com/cmutel/constructive_geometries

Regionalization-examples

The most recent version of the Jupyter notebook files for the case study, as well as more examples of regionalized LCIA calculations, can be found at <https://github.com/cmutel/regionalized-lca-examples>.

Using density (value per area) instead of value

It is important to use densities (e.g. population density) instead of absolute values (e.g. population count) in the L and X matrices. Consider the following example:



In this case, using population count would give a much higher weight to b_2 than b_1 , even though the actual population in $a_1 \cap b_1$ and $a_1 \cap b_2$ are the same (assuming equal population distribution in the (single) spatial unit of A). We have a generic equation for a weighted and normalised spatial intersection:

$$N_{ABAB}$$

If we use population counts:

$$N_{ABAB} = \left(\frac{1}{17} \right) \left(1 \quad 1 \right) \begin{pmatrix} 1 \\ 16 \end{pmatrix} = \left(\frac{1}{17} \quad \frac{16}{17} \right)$$

This bias is gone if we use population density:

$$N_{ABAB} = \left(\frac{1}{2} \right) \left(1 \quad 1 \right) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \left(\frac{1}{2} \quad \frac{1}{2} \right)$$

Scientific notebooks (Jupyter)

All case study calculations were done in a series of [Jupyter notebooks](#), which are included in the electronic supporting information in HTML form. The notebooks have instructions on how they should be used.

The notebooks are also available online:

- [1 - Write CFs as JSON with loading](#)
- [2 - Enter and process data](#)
- [3 - LCA calculations](#)

Case study

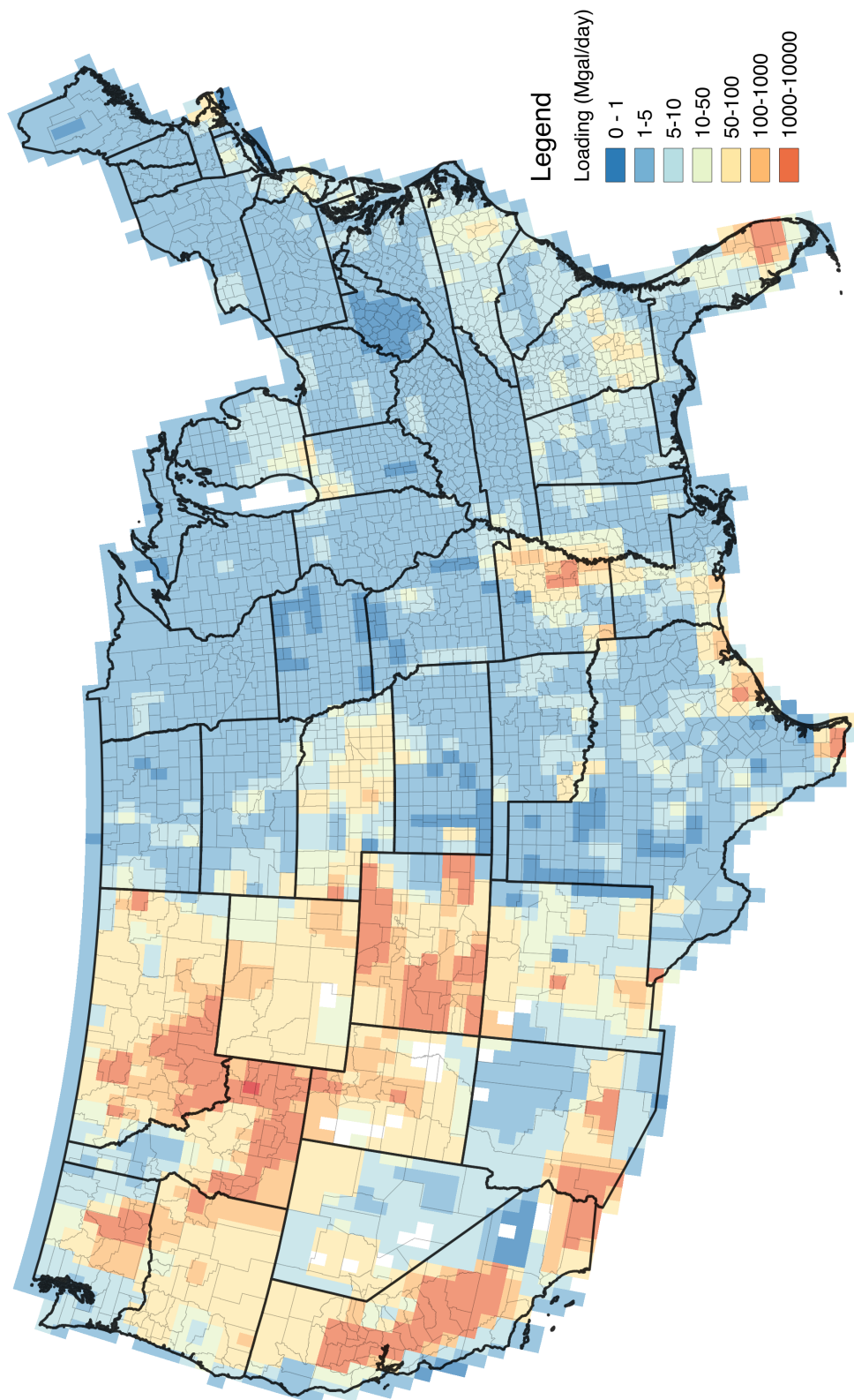


Figure S1: Background loadings for irrigation surface water withdrawal, in millions of gallons per day. Values adapted from USGS county-level data (Kenny, J. F.; Barber, N. L.; Hutson, S. S.; Linsey, K. S.; Lovelace, J. K.; Maupin, M. A. *Estimated Use of Water in the United States in 2005 Circular 1344*. Water 2009, 1344, 52.).

Figure S2: Characterization factors for ecosystem damage due to surface freshwater consumption, in $\text{PDF}\cdot\text{m}^2/\text{yr}/\text{m}^3$.

