Analytical Tools and Algorithms for Life Cycle Assessment

Sangwon Suh[1,2] Reinout Heijungs[2]

[1] University of Minnesota

[2] CML, Leiden University, the Netherlands

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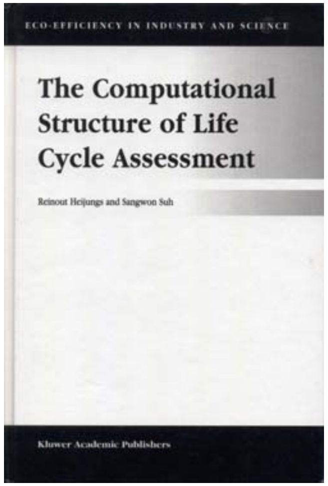
- Introduction
- Analytical tools and algorithms and their applications
  - Theory
  - Updates
  - Application
- Discussions and Outlook

I. Introduction



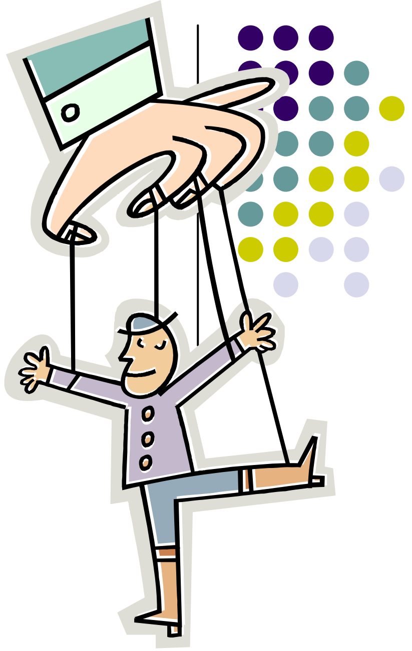
- Matrices: learned once in our life time.
- LCA software tools: what's behind?
- The Computational Structure of Life Cycle Assessment, Kluwer Academic Publisher (2002).
- These tools and algorithms are useful not only for designing software tools but for an efficient interpretation of LCA results.
- Objectives:
  - Review a set of selected tools and algorithms
  - Update with recent findings
  - Outlook
- Will not deal with technical details.

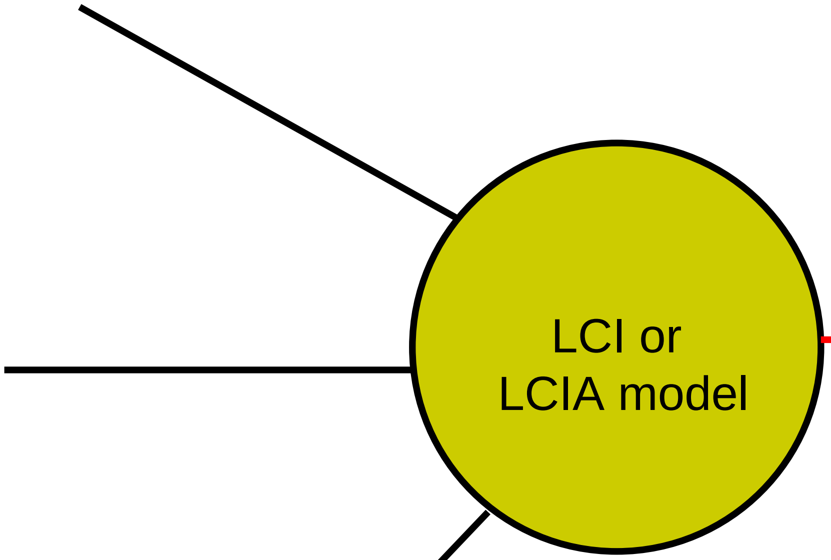
II. Tools and algorithms

- Perturbation theory and key issue identification method
- Input and Output contribution analyses
- Solving the “thickness” problem
- Computation algorithms for allocation

II. 1. Perturbation theory and key issue identification method

Perturbation theory





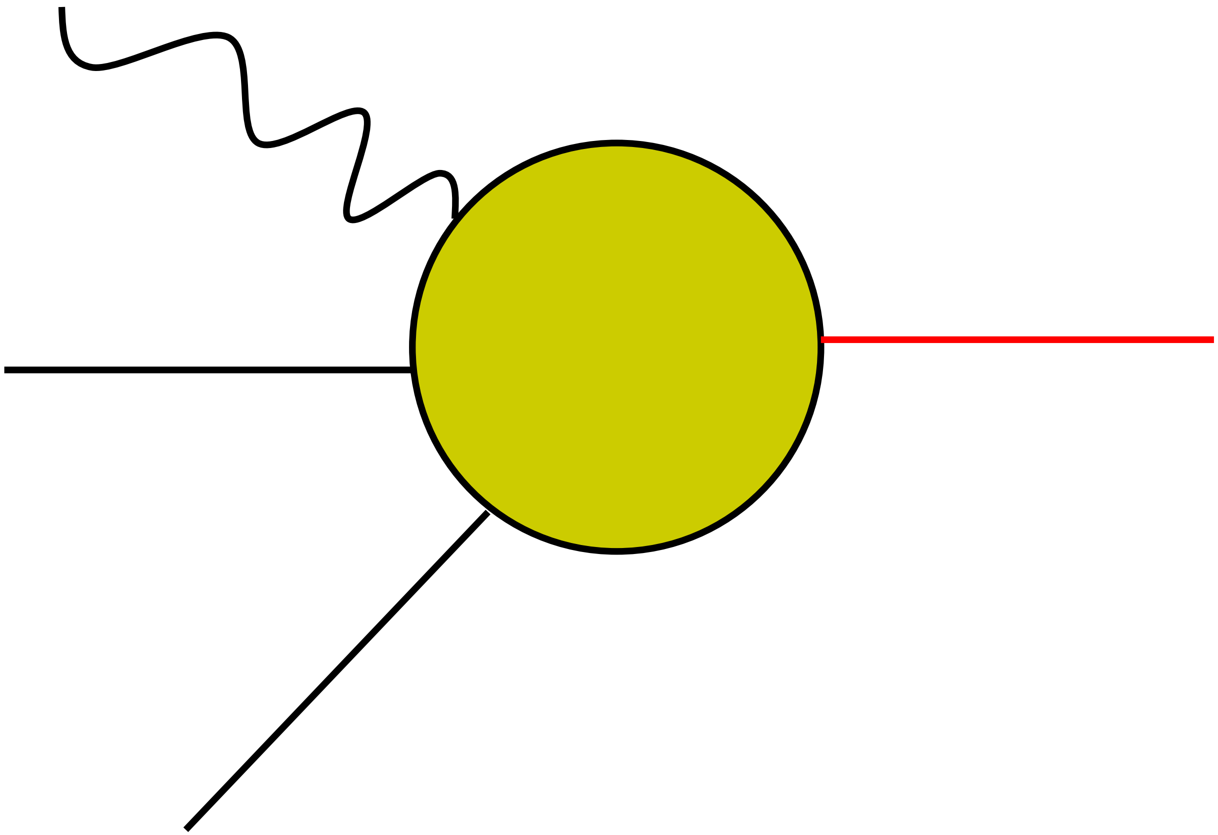
Model output

- LCI results
- LCIA results

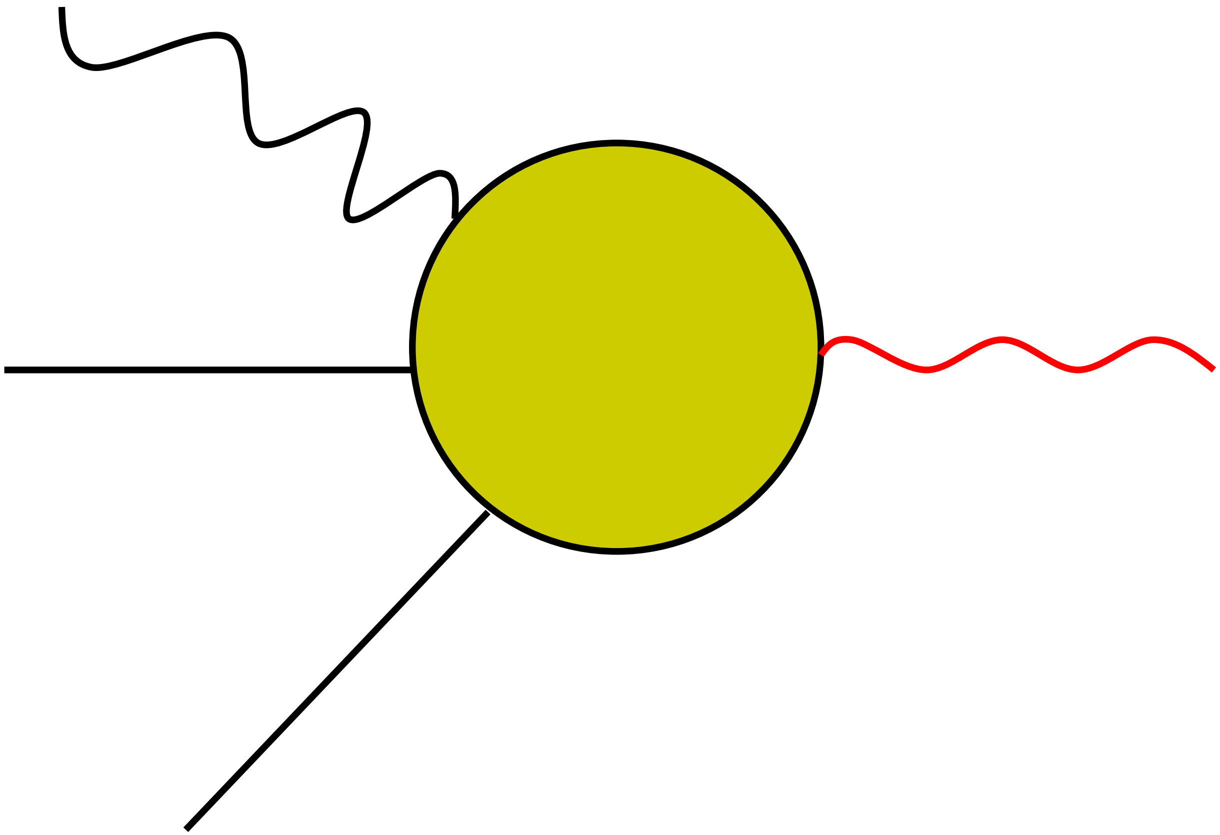
Input parameters

- Input/Output ratio of unit processes
- Characterization factors
- Weighting factors
- etc.

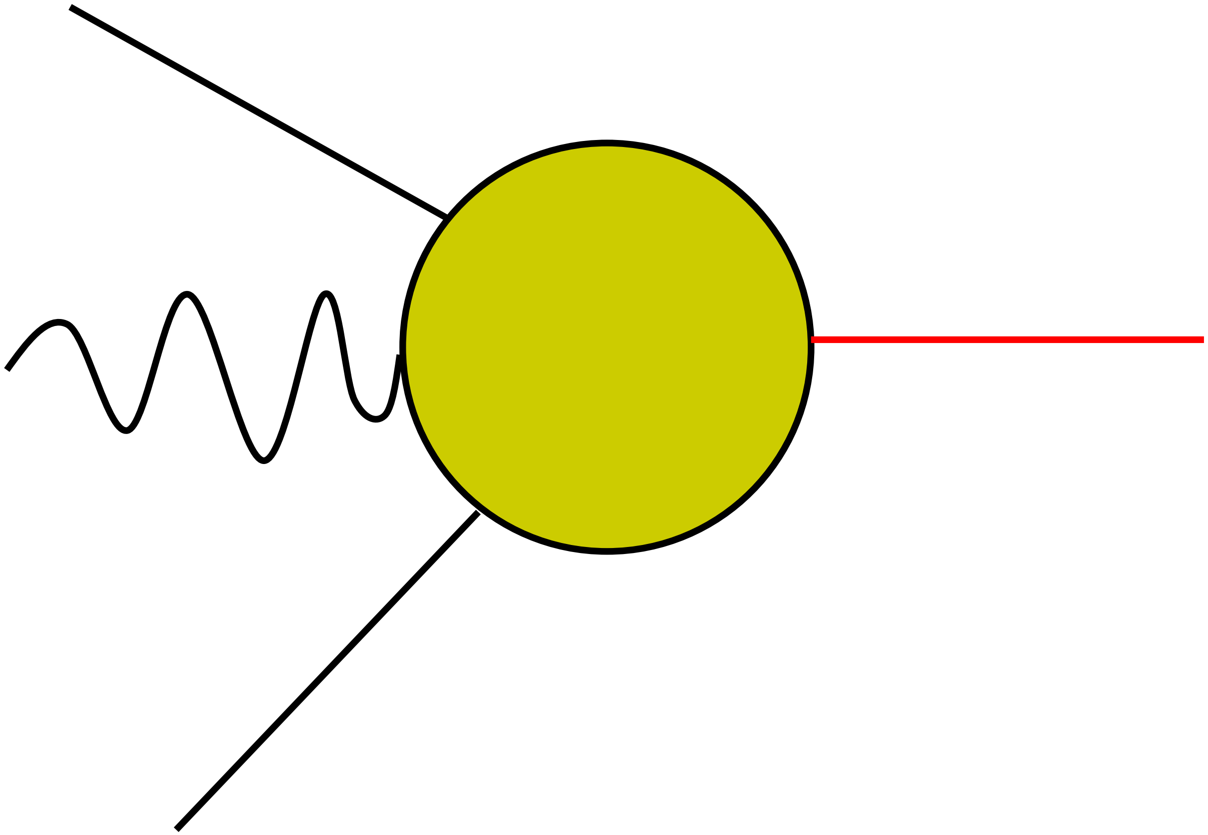
Perturbation theory



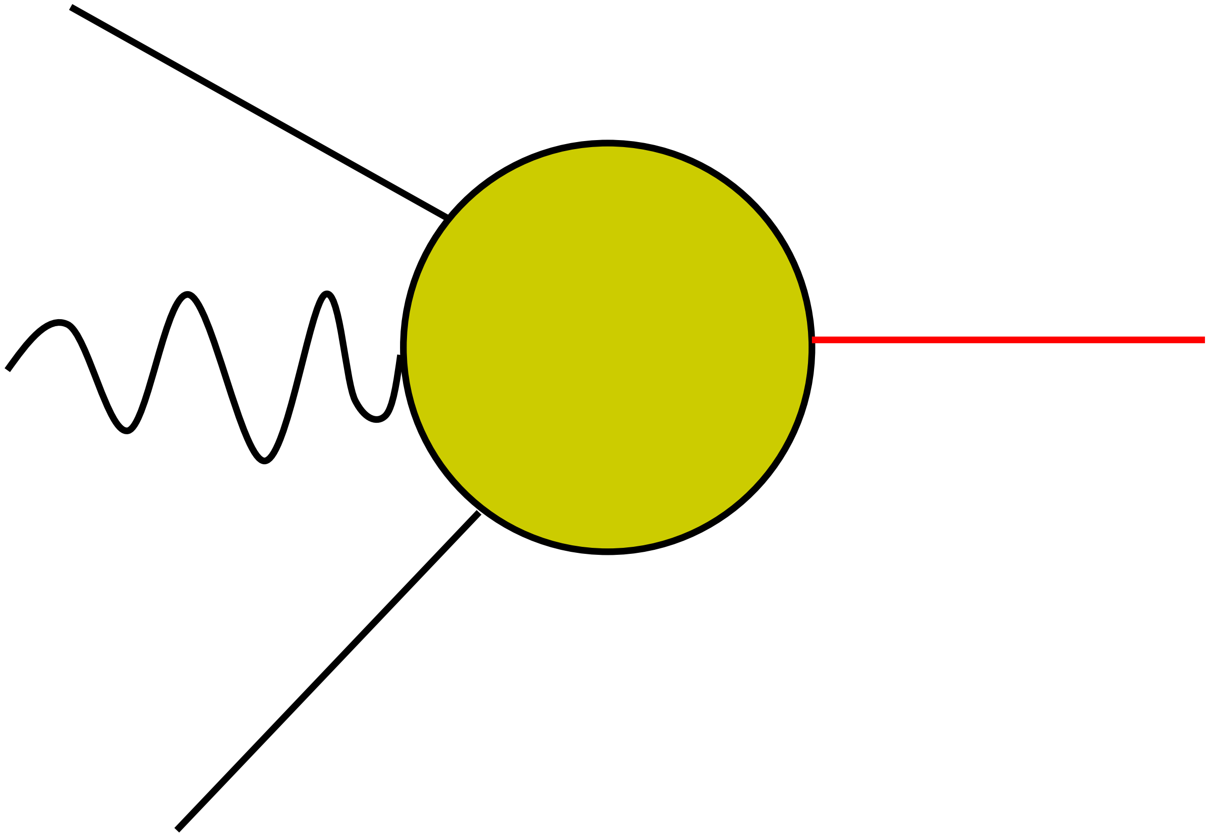
Perturbation theory



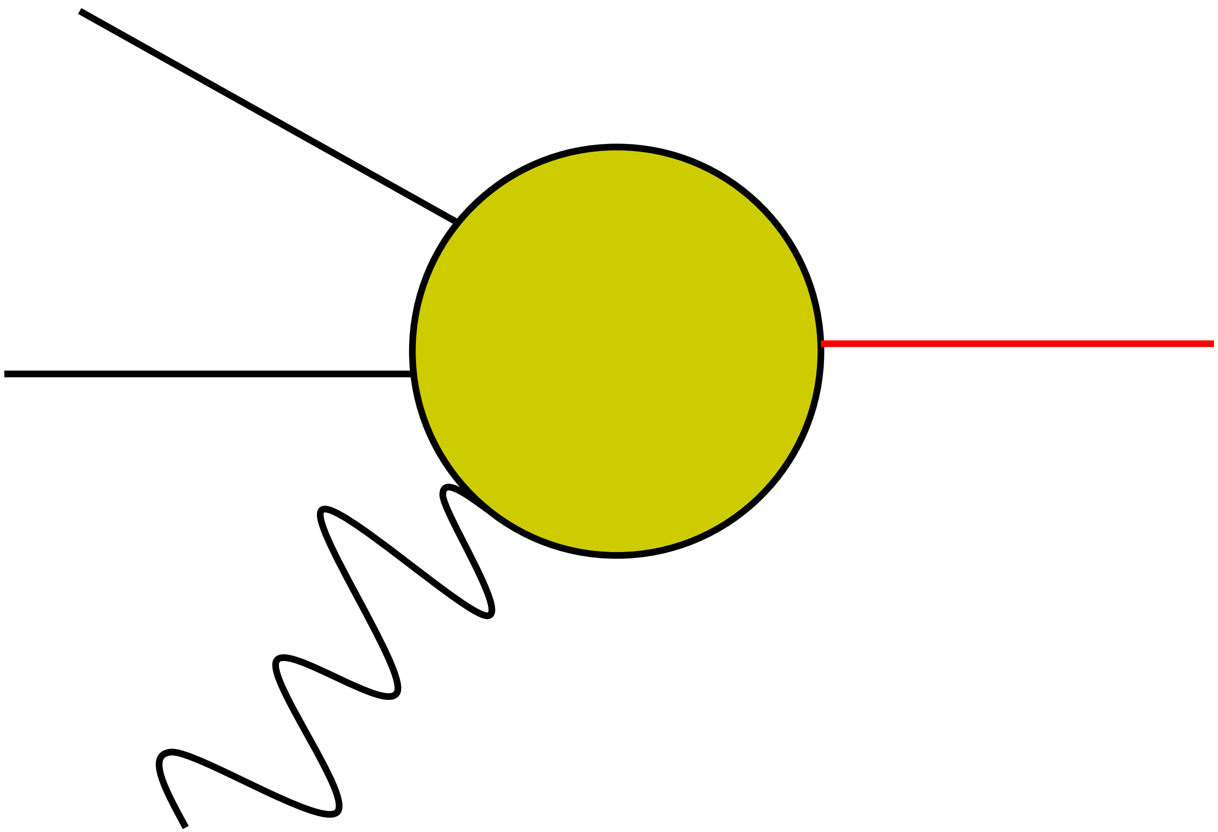
Perturbation theory



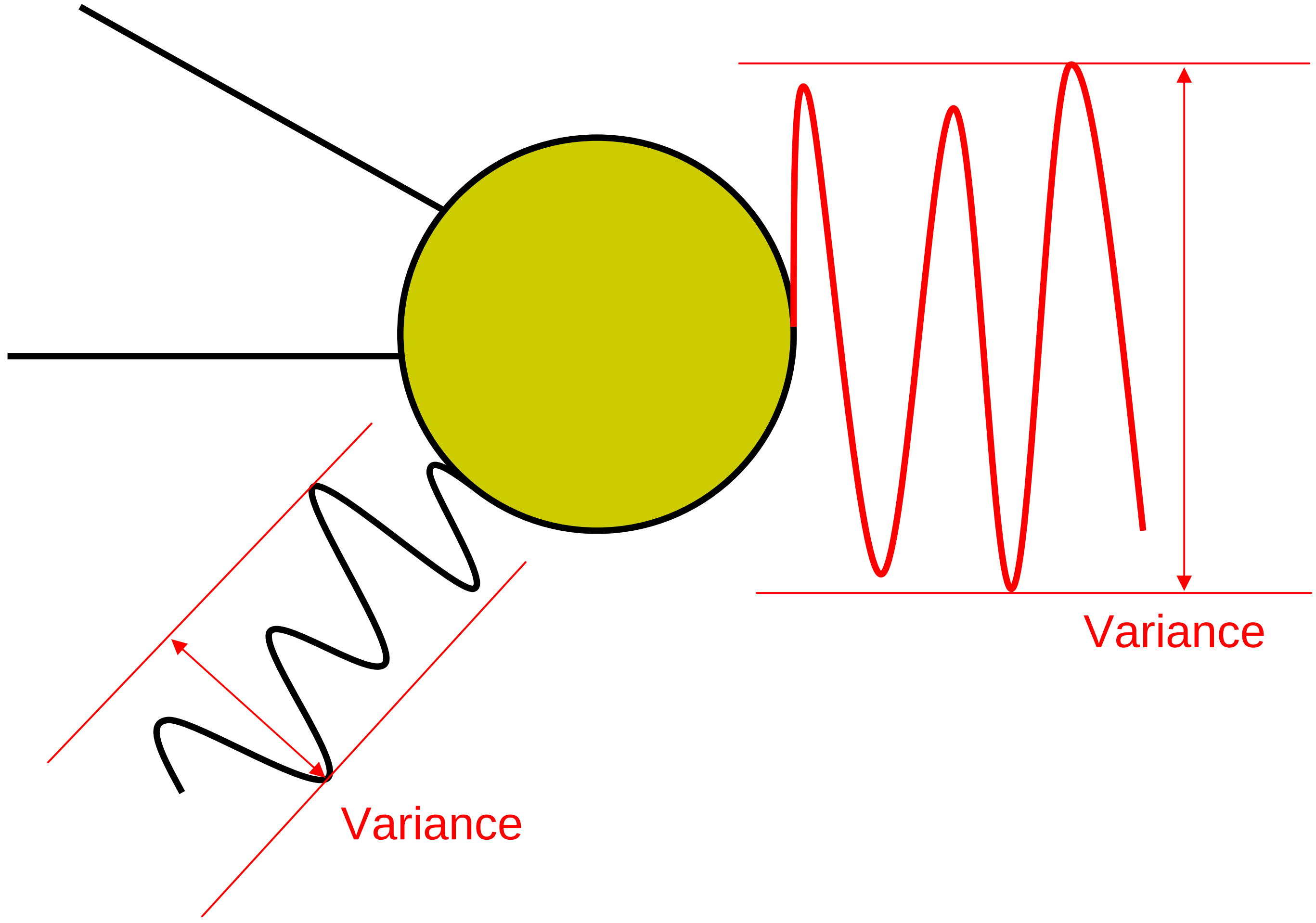
Perturbation theory



Perturbation theory



Perturbation theory



Perturbation of input/output ratio of a unit process

- Heijungs and Suh (2002).

$$\mathbf{A}\mathbf{s} = \mathbf{f}$$

$$(\mathbf{A} + \delta\mathbf{A})(\mathbf{s} + \delta\mathbf{s}) = \mathbf{f}$$

$$\Leftrightarrow \mathbf{A}\delta\mathbf{s} + \delta\mathbf{A}\mathbf{s} + \delta\mathbf{A}\delta\mathbf{s} = \mathbf{0}$$

$$\Leftrightarrow (\mathbf{A} + \delta\mathbf{A})\delta\mathbf{s} = -\delta\mathbf{A}\mathbf{s}$$

$$\Leftrightarrow \delta\mathbf{s} = -(\mathbf{A} + \delta\mathbf{A})^{-1}\delta\mathbf{A}\mathbf{s}$$

$$\Leftrightarrow \delta\mathbf{s} = -(\mathbf{A} + \delta\mathbf{A})^{-1}\delta\mathbf{A}\mathbf{A}^{-1}\mathbf{f}$$

$$\delta\mathbf{s} = -(\mathbf{A} + \delta\mathbf{A})^{-1}\delta\mathbf{A}\mathbf{A}^{-1}\mathbf{f} \; {}^{*}$$

$$\Leftrightarrow \frac{\partial\mathbf{s}}{\partial a_{ij}} = -\frac{\mathbf{A}^{-1}\partial\mathbf{A}\mathbf{A}^{-1}\mathbf{f}}{\partial a_{ij}}$$

$$\Leftrightarrow \frac{\partial\mathbf{s}}{\partial a_{ij}} = -\frac{\partial(\mathbf{A}^{-1})\mathbf{f}}{\partial a_{ij}}$$

$$\boxed{\Leftrightarrow \frac{\partial s_k}{\partial a_{ij}} = -(\mathbf{A}^{-1})_{ki}\, s_j}$$

* Assuming that $\mathbf{A} + \delta\mathbf{A} = \mathbf{A}$

Updates

- Sherman and Morrison equation

$$((\mathbf{A}+\delta\mathbf{A})^{-1})_{kl} = (\mathbf{A}^{-1})_{kl} - \frac{(\mathbf{A}^{-1})_{ki}(\mathbf{A}^{-1})_{jl}\,\Delta a_{ij}}{1+(\mathbf{A}^{-1})_{ji}\,\Delta a_{ij}}$$

$$\Leftrightarrow \frac{((\mathbf{A}+\delta\mathbf{A})^{-1})_{kl} - (\mathbf{A}^{-1})_{kl}}{\Delta a_{ij}} = -\frac{(\mathbf{A}^{-1})_{ki}(\mathbf{A}^{-1})_{jl}}{1+(\mathbf{A}^{-1})_{ji}\,\Delta a_{ij}}$$

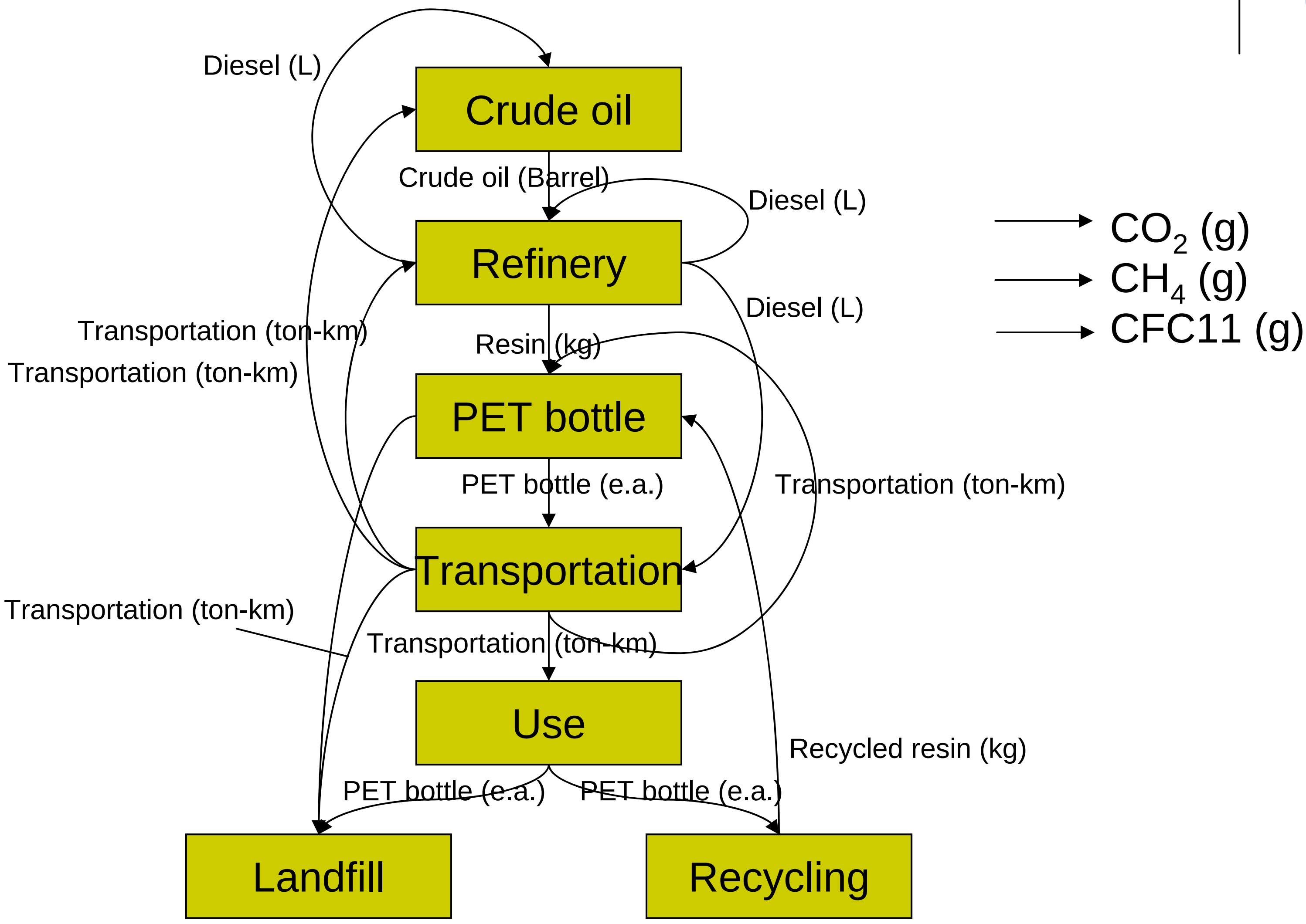
$$\ldots \qquad \boxed{\frac{\Delta s_k}{\Delta a_{ij}} = \frac{-(\mathbf{A}^{-1})_{ki}\,s_j}{1+(\mathbf{A}^{-1})_{ji}\,\Delta a_{ij}}}$$

- Exact solutions of a perturbation problem without using the first order approximation possible.

When do the two make a difference?

- Generally the first order approximation and the Sherman-Morison approach generate almost identical results, unless:
- $(\mathbf{A}^{-1})_{ji}\Delta a_{ij}$ is large in absolute value.
- I.e., direct input of *i* for producing *j* has large variance + producing *i* requires *j* in large quantity directly and indirectly.

Application



Application

	Crude oil extraction	Refinery (resin)	Refinery (fuel)	PET bottle manufacturing	Transportation	Use	Recycl ing	Landfill
Crude oil (Barrel)	1	-1	-1	0	0	0	0	0
Resin (kg)	0	5	0	-0.03	0	0	0	0
Diesel (L)	-7	-0.1	40	-0.001	-1.2	0	-0.5	0
PET bottle (e.a.)	0	0	0	1	0	-1	0	0
Transportation (ton-km)	- 200	-6.4	5.3	-0.001	25	-0.0002	-1.1	-0.02
Use of 1.5L PET bottle (e.a.)	0	0	0	0	0	1	-1000	0
Recycled resin (kg)	0	0	0	-0.01	0	0	32.4	0
Landfill service (kg)	0	0	0	-0.02	-0.002	-0.04	-11	1
CO_2 (g)	750	340	2100	25.4	2680	0	1.36	0
CH_4 (g)	230	0.1	0.2	0.03	0	0	0	0
CFC11 (g)	0	0	0	0.001	0.003	0	0	0

Application

- Standard deviation

	Crude oil extraction	Refinery (resin)	Refinery (fuel)	PET bottle manufacturing	Transportation	Use	Recycl ing	Landfill
Crude oil (Barrel)	0	0.4	0.02	0	0	0	0	0
Resin (kg)	0	0	0	0.01	0	0	0	0
Diesel (L)	0.8	0.05	0	0.0001	0.1	0	0.3	0
PET bottle (e.a.)	0	0	0	0	0	0	0	0
Transportation (ton-km)	27	1.1	0.6	0.0001	0	0.002	0.3	0.03
Use of 1.5L PET bottle (e.a.)	0	0	0	0	0	0	0	0
Recycled resin (kg)	0	0	0	0.005	0	0	0	0
Landfill service (kg)	0	0	0	0.001	0.004	0.01	3.6	0

Application

- Sensitivity (1% homogeneous change)

	Crude oil extraction	Refinery (resin)	Refinery (fuel)	PET bottle manufacturing	Transport-ation	Use	Recycling	Landfill
Crude oil (Barrel)	0.0077	0.0043	0.0032	0	0	0	0	0
Resin (kg)	0	0.0045	0	0.0045	0	0	0	0
Diesel (L)	0.0014	0	0.0035	0	0.0020	0	0	0
PET bottle (e.a.)	0	0	0	0.0073	0	0.0071	0	0
Transportation (ton-km)	0.0052	0.0001	0.0001	0	0.0054	0	0	0
Use of 1.5L PET bottle (e.a.)	0	0	0	0	0	0.0073	0.0022	0
Recycled resin (kg)	0	0	0	0.0022	0	0	0.0022	0
Landfill service (kg)	0	0	0	0	0	0	0	0

Application

- Contribution to the overall variance of the Characterization results (Global warming)

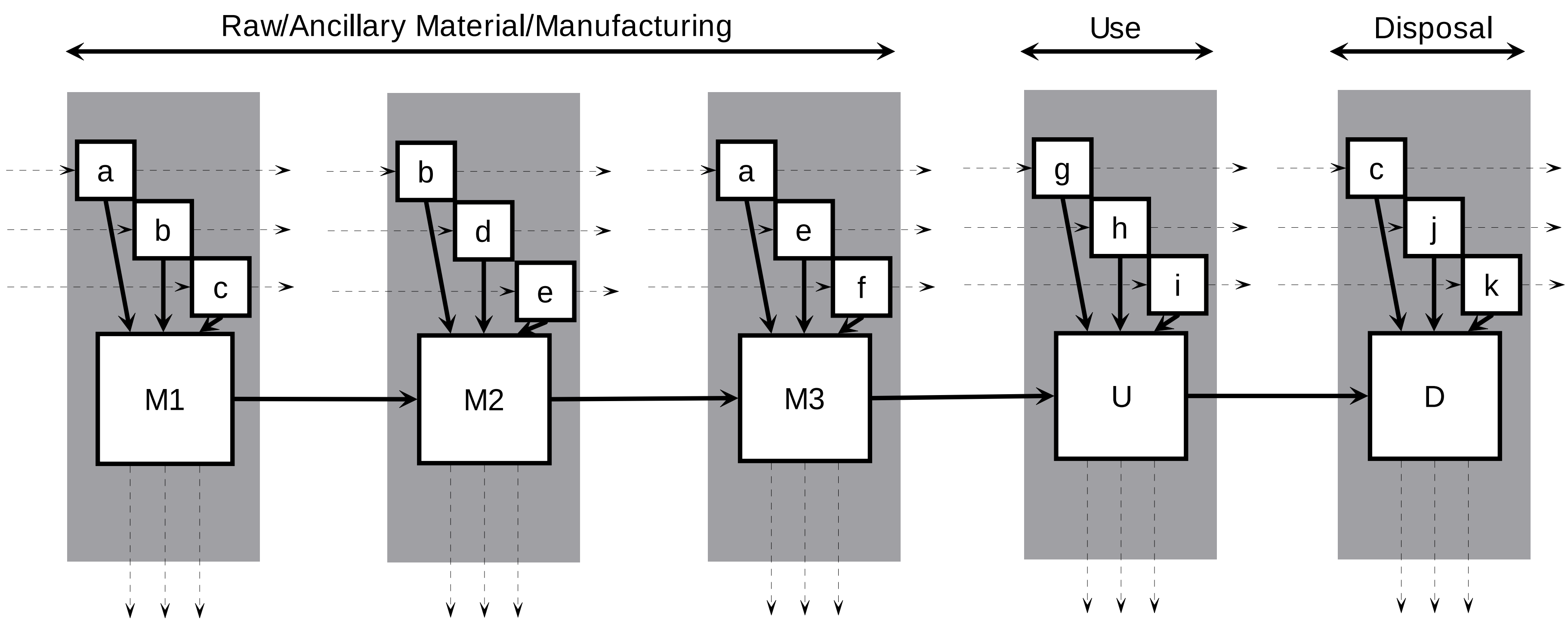
	Crude oil extraction	Refinery (resin)	Refinery (fuel)	PET bottle manufacturing	Transport-ation	Use	Recycling	Landfill
Crude oil (Barrel)	0.00	0.43	0.00	0.00	0.00	0.00	0.00	0.00
Resin (kg)	0.00	0.00	0.00	0.32	0.00	0.00	0.00	0.00
Diesel (L)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PET bottle (e.a.)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Transportation (ton-km)	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Use of 1.5L PET bottle (e.a.)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Recycled resin (kg)	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00
Landfill service (kg)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

II. 2. Input and output contribution analyses

Structuring issue

- Two main structuring options:
  - What are the most important (sub)process(es) in the product system?
    - Ex) Which process in the entire life cycle of a product generated the most of CO_2?
  - What are the most important input material(s) in the product system?
    - Ex) Which direct input material induced the direct and supply-chain CO_2 emission the most (embodied emission)?

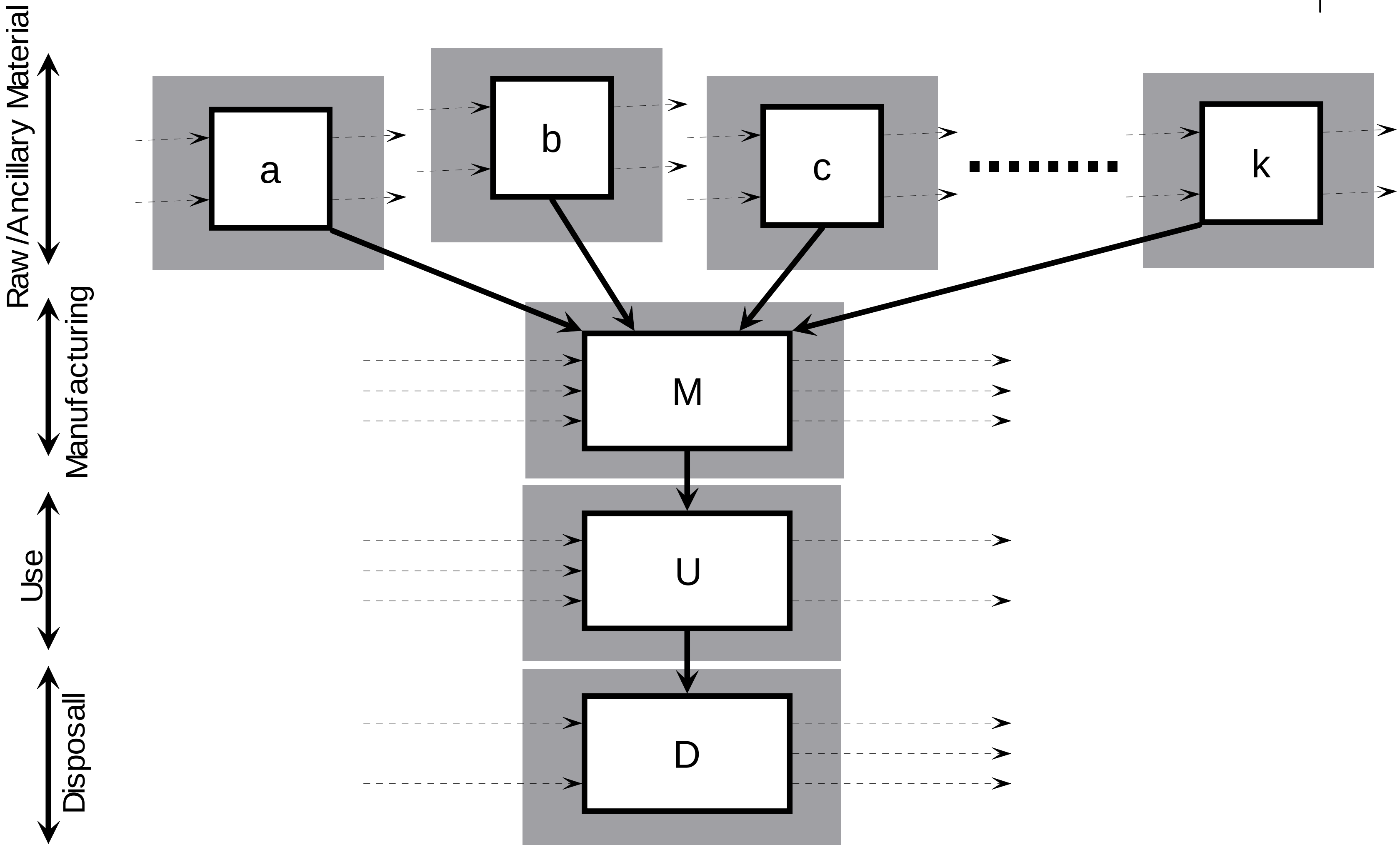
Key (sub) process



Flow of (intermediate) products

Flow of environmental

Key raw and ancillary material



Input and Output Contribution Analysis

- Input contribution analysis:
  - Identifies direct inputs that induce most of the environmental impacts.
  - $\mathbf{h}_k^{\Omega} = (\widehat{\mathbf{CB}})_{k.}\mathbf{A}^{-1}\mathbf{f}$
- Output contribution analysis:
  - Identifies processes in the product's life cycle that generate most of the environmental impacts.
  - $\mathbf{h}_k^{\mathrm{A}} = (\mathbf{CB})_{k.}\mathbf{A}^{-1}(\widehat{((\mathbf{I}-\mathbf{A})\mathbf{f}})$

Applications

- In 1998, hospitals have generated 268.3Tg CO_2-equiv Greenhouse gases.*
- Where were these emissions directly occurred (output contribution)?
  - Electricity (37.0%); Sanitary services and steam supply (7.7%); Agricultural products (4.5%); Crude petroleum and natural gas (3.8%); Blast furnaces and steel mills (3.0%); Air transportation (2.8%); Plate making and related services (2.7%); Construction and maintenance (2.5%).

* Suh, S. 2006: Are Services Better for the Climate Change? Environmental Science & Technology.

Applications

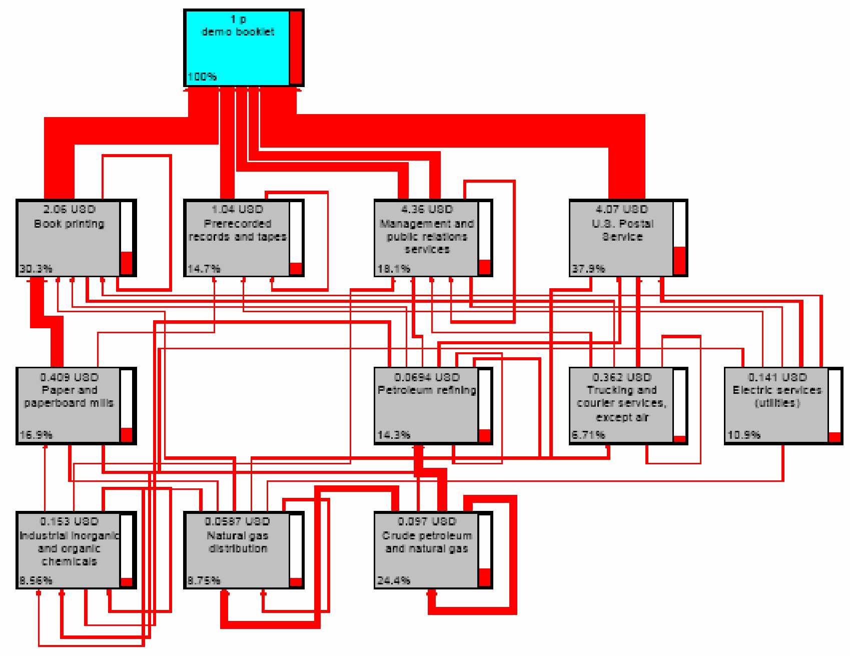
- In 1998, hospitals have generated 268.3Tg CO_2-equiv Greenhouse gases.*
- Which direct inputs did induce these emissions (input contribution)?
  - Electricity (25.5%); Real estate agents (6.4%); Sanitary services and steam supply (5.1%); Organic and inorganic chemicals (5.0%); Industrial and commercial buildings (4.4%); Drugs (3.5%); Surgical and medical instruments and apparatus (2.1%); Surgical appliances and supplies (1.9%).

* Suh, S. 2006: Are Services Better for the Climate Change? Environmental Science & Technology.

II. 3. Solving the “thickness” problem

“Thickness” problem

- Visualization of direct and indirect contributions between processes
- Can be complicated for larger systems



A screen shot of SimaPRO

Ecological network analysis

- Environ analysis: B. Patten (1982)*
  - Output Environ analysis
  - $\mathbf{E}^{\Omega,k} = \hat{\mathbf{N}}^{**}_{.k}\mathbf{Q}^{**}$
- More efficient calculus: Suh (2005)**
  - $\mathbf{E}^{\Omega,i} = \overline{\hat{\mathbf{D}}}_{i.}\overline{\mathbf{A}}$
  - Or more simply with scalar notation:
  - $e^{\Omega,k}_{ij} = \overline{d}_{ki}\overline{a}_{ij}$

* Patten,B.C., 1982. Environs - Relativistic Elementary-Particles for Ecology. *American Naturalist*
** Suh, S., 2005. Theory of Materials and Energy Flow Analysis in Ecology and Economics. *Ecological Modeling*

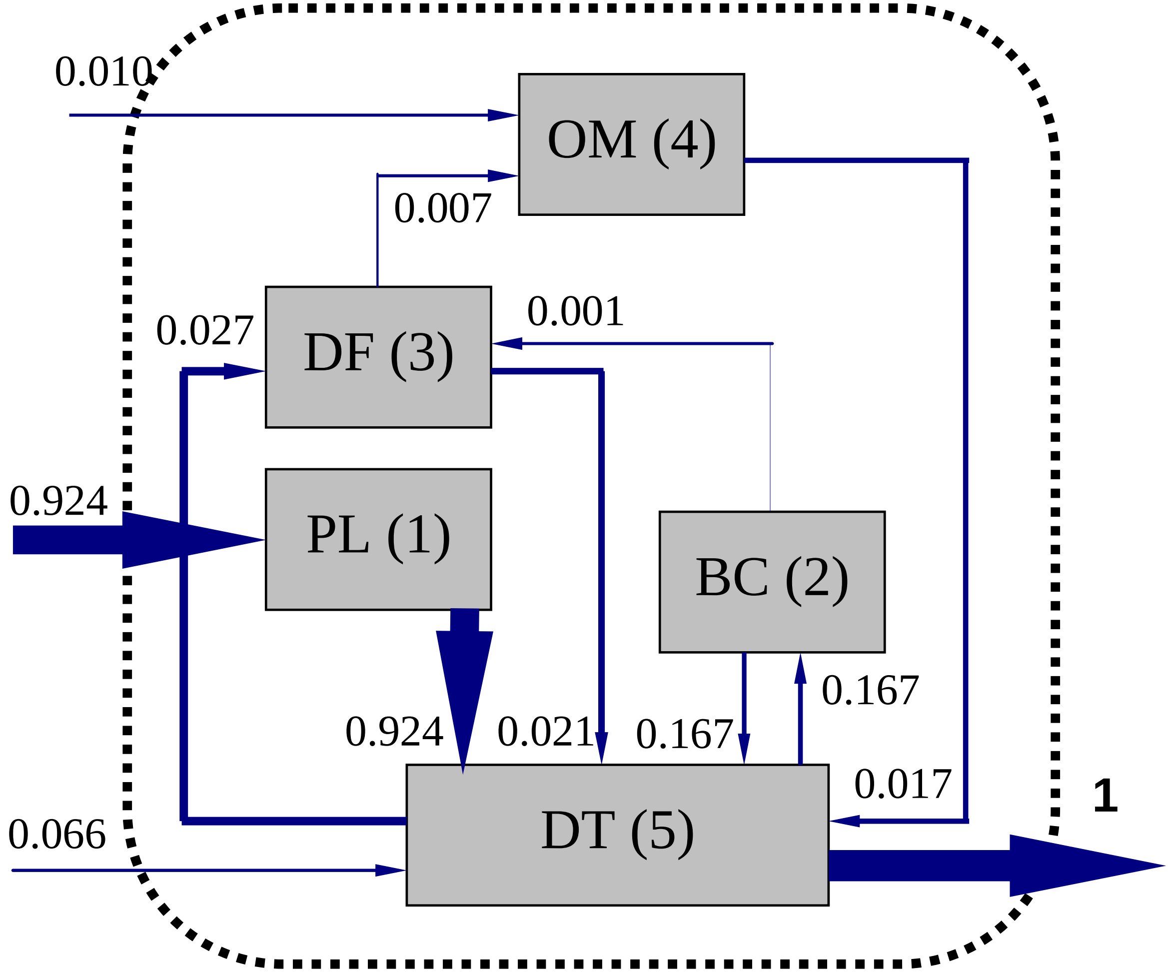
Application

- Energy Input-Output data of Cone Spring ecosystem

	(1)	(2)	(3)	(4)	(5)	Exports (y)	Respiration (r)	Changes in stock (s)	Total Production (x)
(1) Plants	0	0	0	0	8881	300	2003	-200	10984
(2) Bacteria	0	0	75	0	1600	255	3275	0	5205
(3) Detritus feeders	0	0	0	370	200	0	1814	0	2384
(4) Omnivores	0	0	0	0	167	0	203	500	870
(5) Detritus	0	5205	2309	0	0	860	3109	0	11483
Primary input of bread (w_1)	0	0		500	0				
Primary input of sunlight (w_2)	10984	0	0	0	635				
Total Production (x')	10984	5205	2384	870	11483				

Application

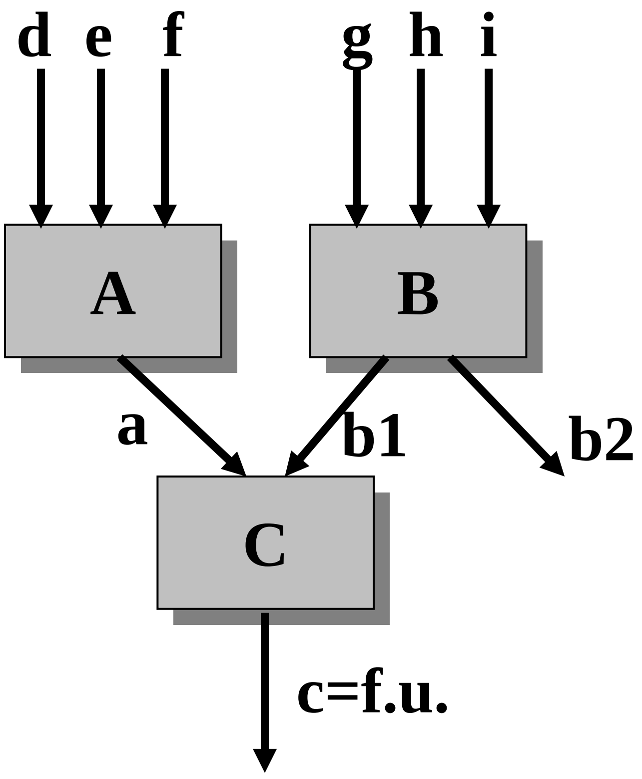
- Visual expression



II. 4. Allocation

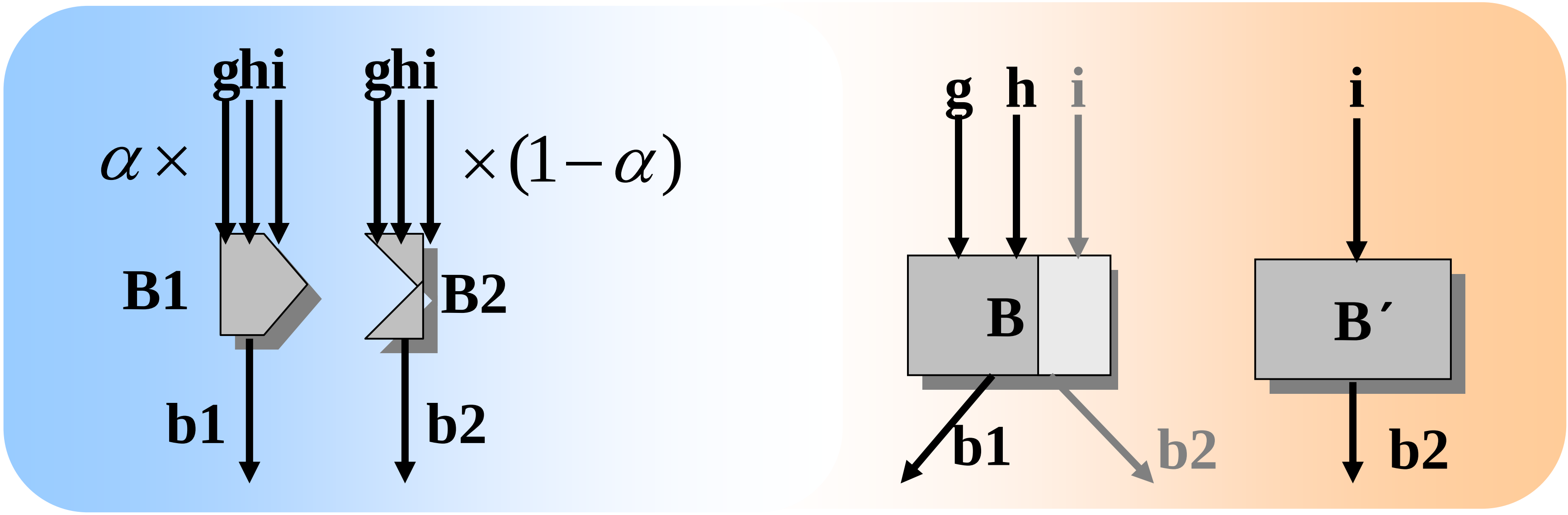
Partitioning and System Expansion

Allocation situation



Partitioning and System Expansion

Partitioning **System expansion**



Example

	Refinery	Electricity	Co-generation	District heating	…
Diesel fuel (MJ)	100	-80	-8	-50	…
Gasoline (MJ)	50	0	0	0	…
Electricity (kWh)	0	10	1	0	…
Steam(MJ)	-20	0	5	5	…
Heat (MJ)	0	5	0	20	…
…					

Example: Endless regression problem (Ekvall and Finnveden (2001), Weidema (2001)

	Refinery	Electricity	Co-generation	District heating	…
Diesel fuel (MJ)	100	-80	-8	-50	…
Gasoline (MJ)	50	0	0	0	…
Electricity (kWh)	0	10	1		…
Steam(MJ)	-20	0	5	5	…
Heat (MJ)	0	5	0	20	…
…					

Mathematical formalism for allocation

V^p U^p U^e

$$\mathbf{V} = \left(\begin{array}{r|rrr} 100 & 0 & 0 & 0 \\ 50 & 0 & 0 & 0 \\ \hline 0 & 10 & 1 & 0 \\ 0 & 0 & 5 & 5 \\ 0 & 5 & 0 & 20 \end{array}\right) \qquad \mathbf{U} = \left(\begin{array}{r|rrr} 0 & 80 & 8 & 50 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 20 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right)$$

V^e

$$\mathbf{V}^{\mathrm{p}} = \begin{pmatrix} 100 & 50 \end{pmatrix}' \qquad \mathbf{U}^{\mathrm{p}} = \begin{pmatrix} 0 & 0 & 0 & 20 & 0 \end{pmatrix}'$$

Mathematical formalism for allocation

- Partitioning

$$\mathbf{A}^{\mathrm{p}} = \mathbf{U}^{\mathrm{p}}\hat{\mathbf{g}}^{-1}(\mathbf{V}^{\mathrm{p}})'\hat{\mathbf{q}}^{-1}$$

$$\mathbf{A}^{\mathrm{p}} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 20 \\ 0 \end{pmatrix} (1/150)(100 \quad 50)\begin{pmatrix} 1/100 & 0 \\ 0 & 1/50 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0.13 & 0.13 \\ 0 & 0 \end{pmatrix}$$

* Hat (^) denote diagonalized vectors

Mathematical formalism for allocation

- System Expansion

$$\mathbf{A}^{\mathrm{e}} = \mathbf{U}^{\mathrm{e}}(\mathbf{V}^{\mathrm{e}})^{-1}$$

$$= \begin{pmatrix} 80 & 8 & 50 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 10 & 1 & 0 \\ 0 & 5 & 5 \\ 5 & 0 & 20 \end{pmatrix}^{-1} = \begin{pmatrix} 6.8 & 0.2 & 2.4 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Mathematical formalism for allocation

- Allocated technology matrix

$$\overline{\mathbf{A}} = (\mathbf{I} - \mathbf{A}^{c})\,\mathrm{diag}\left(\mathbf{V}^{p} \quad \hat{\mathbf{V}}^{e}\right)$$

$$= \begin{pmatrix} 100 & 0 & -67.8 & -1.2 & -48.8 \\ 0 & 50 & 0 & 0 & 0 \\ 0 & 0 & 10 & 0 & 0 \\ -13.3 & -6.7 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 20 \end{pmatrix}$$

- The merger of the two technology matrices calculates allocated LCI.

C.f.

	Refinery	Electricity	Co-generation	District heating	…
Diesel fuel (MJ)	100	-80	-8	-50	…
Gasoline (MJ)	50	0	0	0	…
Electricity (kWh)	0	10	1	0	…
Steam(MJ)	-20	0	5	5	…
Heat (MJ)	0	5	0	20	…
…					

III. Discussion and Outlook

- A number of computation tools and algorithms that aid LCA are selected and reviewed:
  - Theory
  - Updates
  - Application
- These tools and algorithms are helpful:
  - Solving computational problems
  - Better interpreting the results
- They are all available in the form of Matlab coding and available upon request.

III. Discussion and Outlook

- Lecture materials, exercises and home works around these tools and algorithms have been developed and available (for upper level graduate class).
- These tools can be readily mounted to existing LCA software tools.
- Useful tools and algorithms applicable to LCA have been developed in various disciplines, and they are waiting for innovative reformulations by the LCA community.

Thanks!

For more information, contact:

Sangwon Suh (sangwon@umn.edu)

Assistant Professor

University of Minnesota