Optimization for Sustainable Development

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Definitions

What is *Sustainable Development*?

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- Development that can last forever

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- Development that can last forever
- “Décroissance”

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- Making sure the earth can survive
- Preservation of biodiversity
- Helping Africa

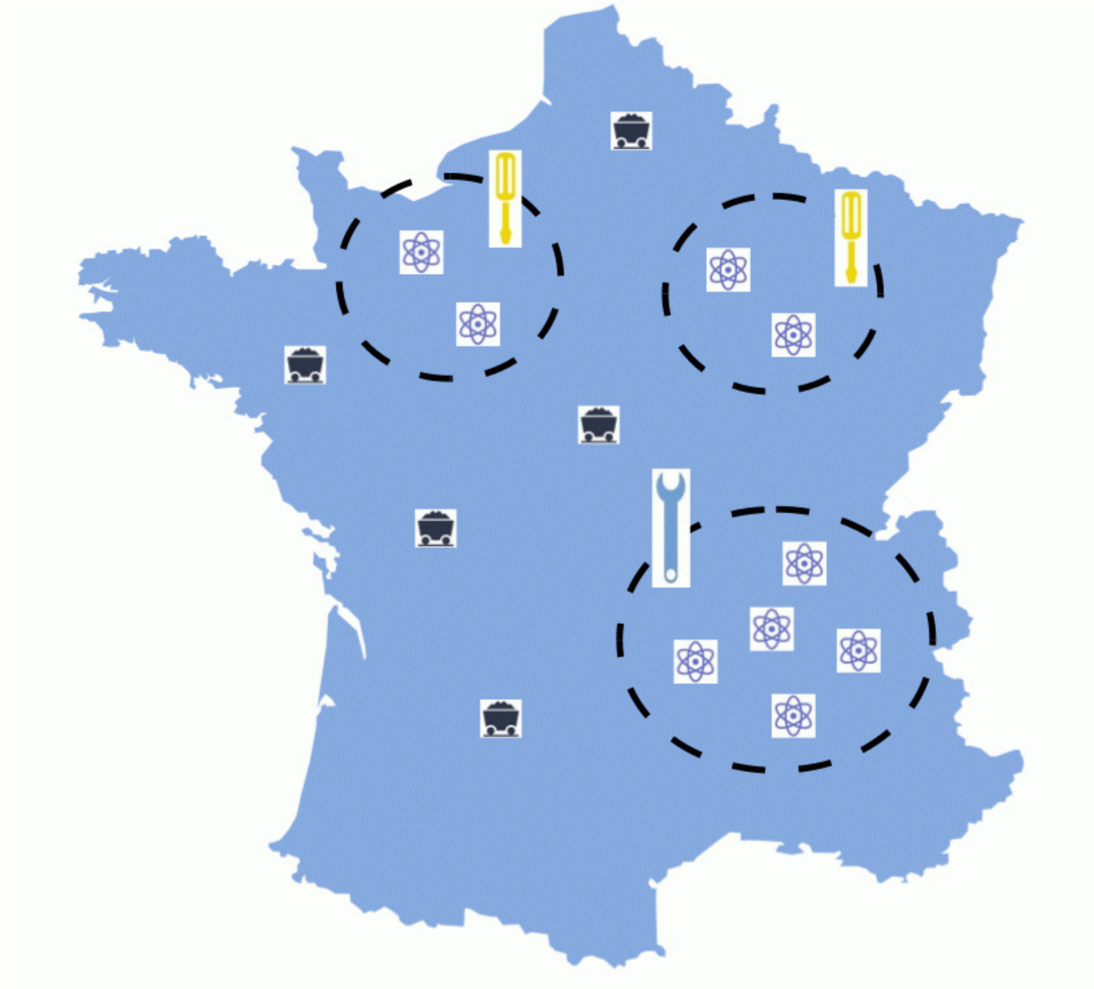
The honest definition

Optimization for Sustainable Development

Set of applications of optimization techniques which also concern the environment

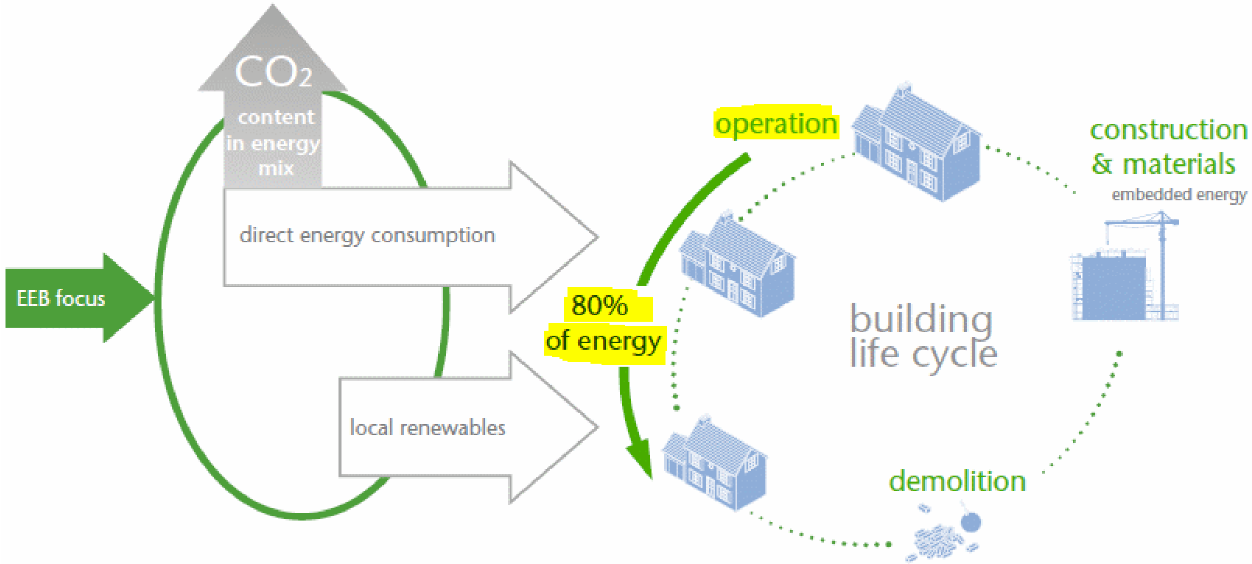
Examples

Scheduling nuclear plant outages



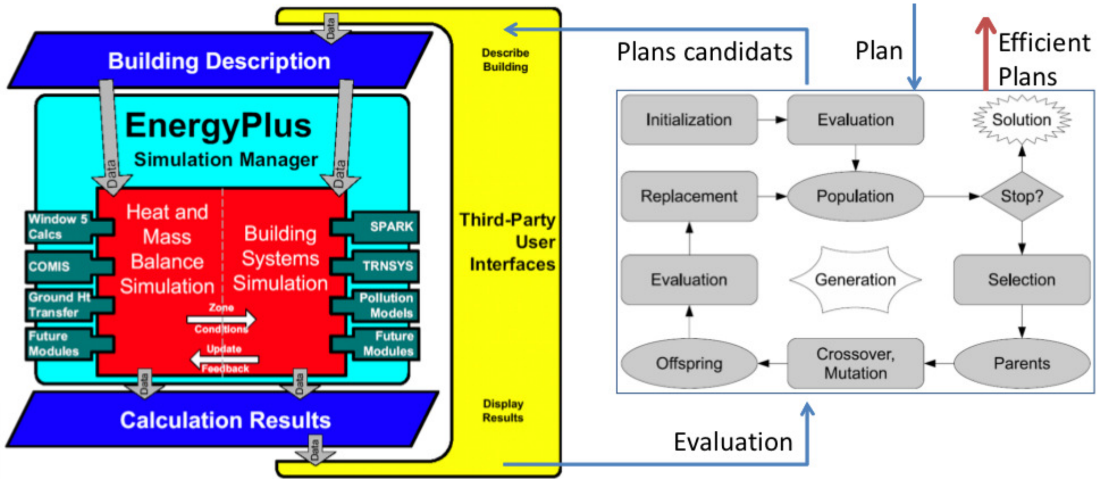
Decide when to shut down nuclear plants subject to technical and demand constraints

Smart buildings

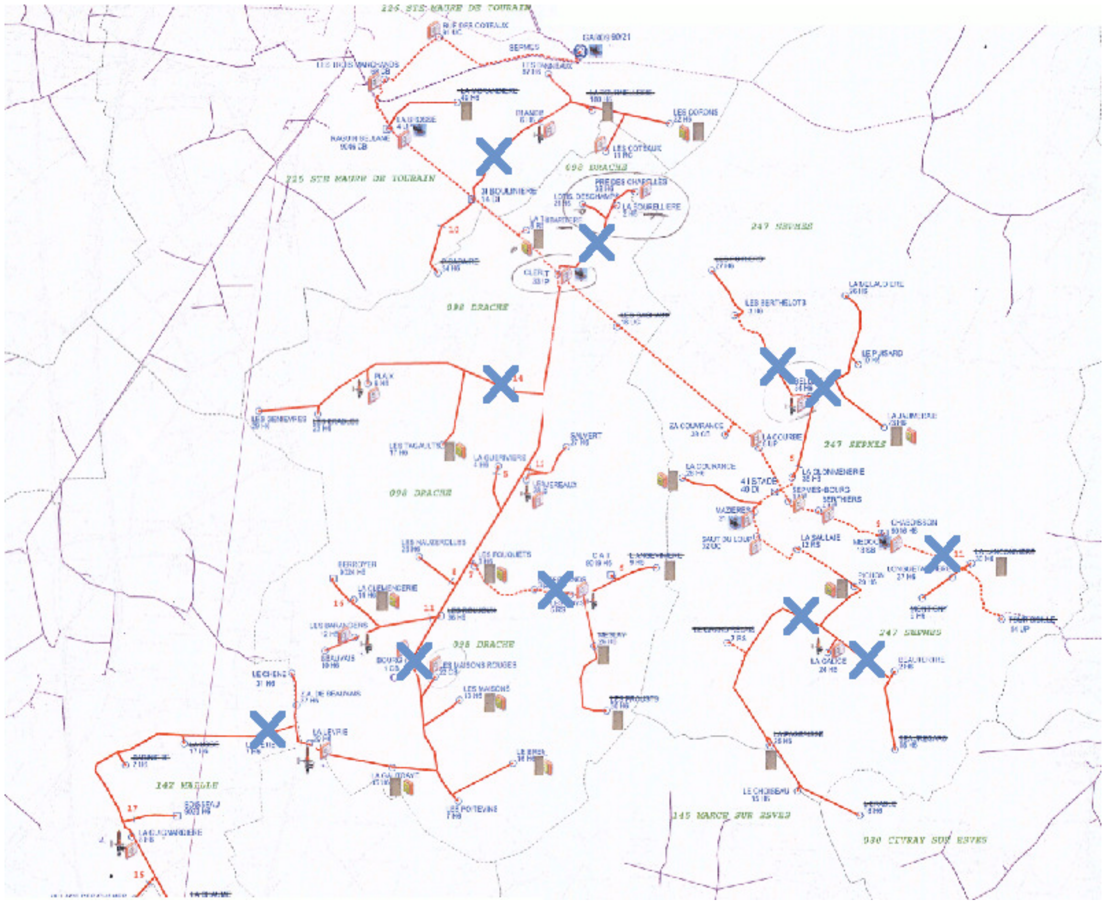


Buildings regulate their temperatures based on climate and smart energy usage

Population-based optimization, evaluate fitness using *EnergyPlus* simulation manager

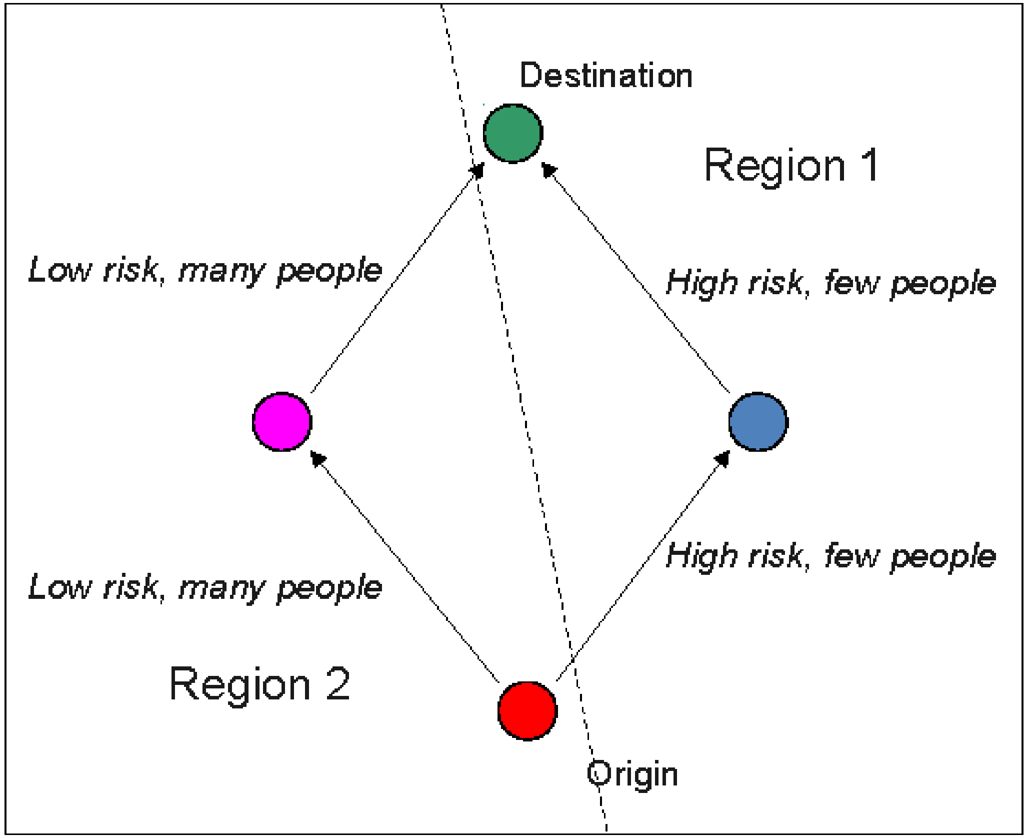


Concentrator placement



Smart grids ⇒ smart meters ⇒ concentrators
Where do we place them? Several technical constraints

Cost of equitability



<u>Decide: quantity of hazmat to route on different roads</u>

Minimize absolute damage:
route everything through region 1

Minimize absolute risk:
route everything through region 2

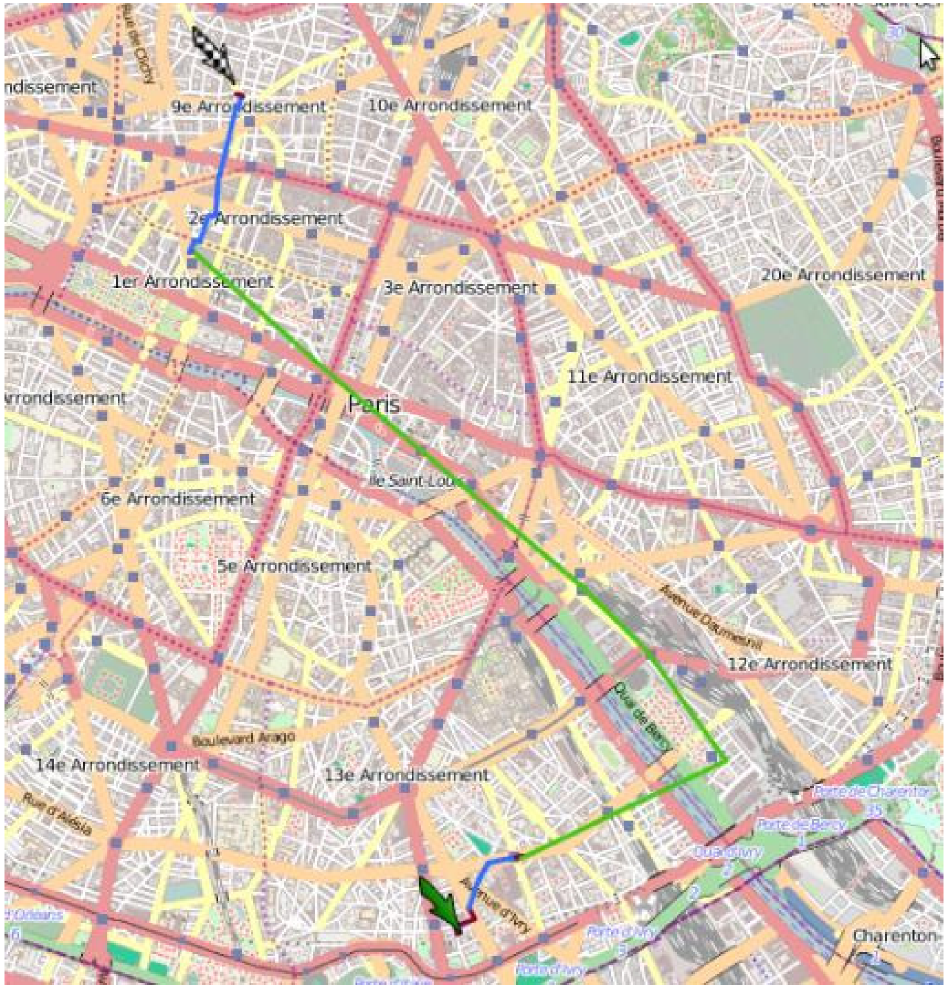
Region equity:
spread risk equally on regions

Rawl's principle:
min. risk of most disadvantaged zone

Equity ≠ Damage:
Can fairness kill more people?

Hazmat transportation regulations often share the risk equitably among different administrative regions: **this may cost lives**

Multifeature shortest paths



Changing vehicles, optimizing time and CO_2 *emissions, passing through given spots*: **used in road network routing devices**

A more precise definition

Sustainability in time

No single definition

How do we propose to use optimization techniques for something that cannot even be defined precisely?

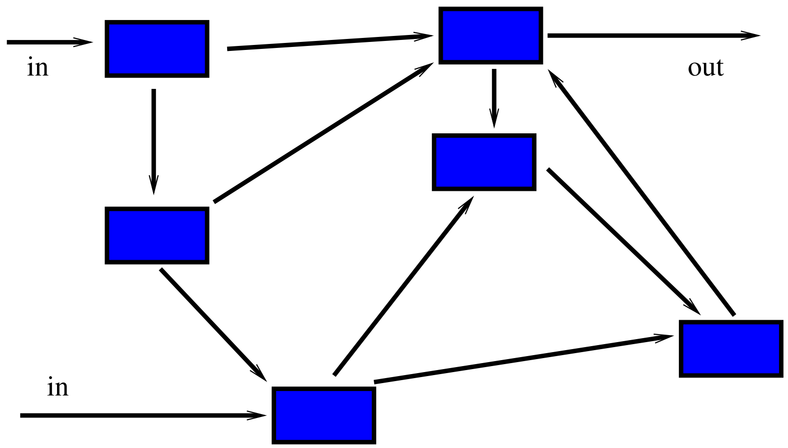
Focus on one aspect

“Development that can last forever”

“Development”: working definition

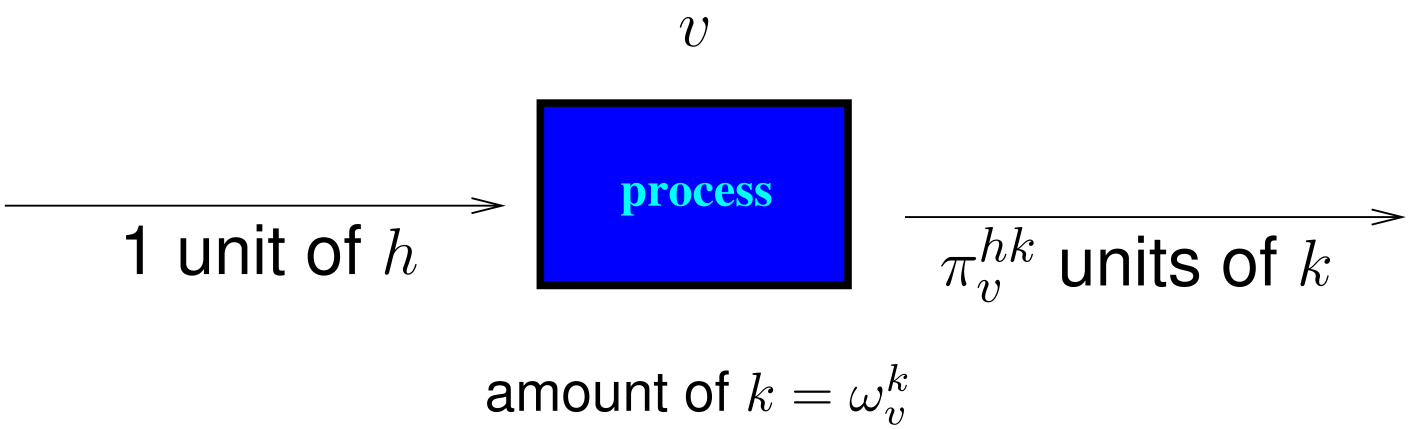
- We define “development” as a set of processes that transform input into output

- *Input/output can be*: mass, energy, information, work, time, value. . .
- These processes can sometimes be decomposed into complex networks of inter-related processes
- Conversely, processes can be combined to form networks



Transformation

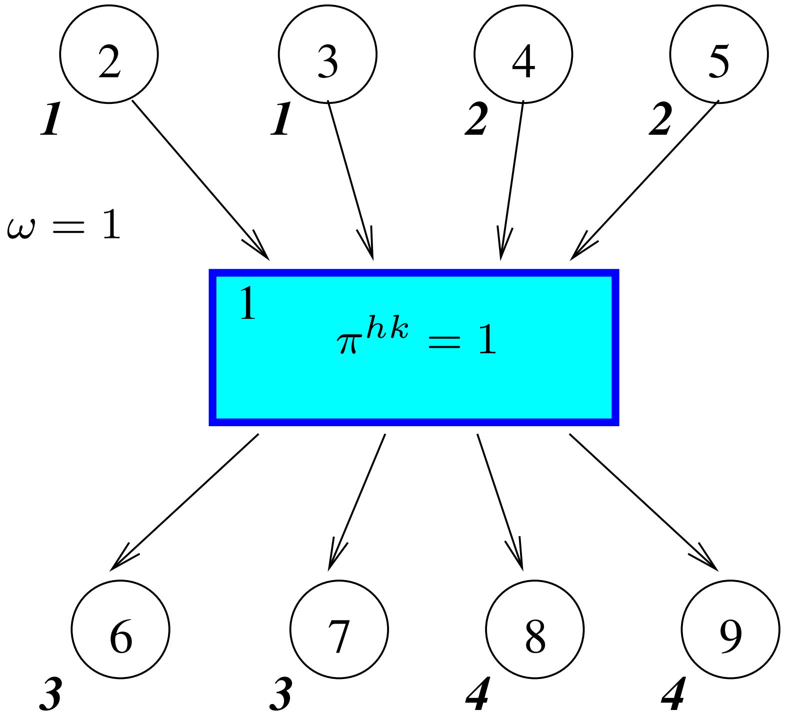
- π_v^{hk}: quantity of k yielded per unit of h transformed by v
- ω_v^k: amount of k stored at v



Unsustainability

Example

Plant 1 draws products **1,2** from inputs 2,3,4,5, transforms **1,2** into 1 unit of **3** and 1 unit of **4**, pushed to outputs 6,7,8,9



Decide flows on arcs

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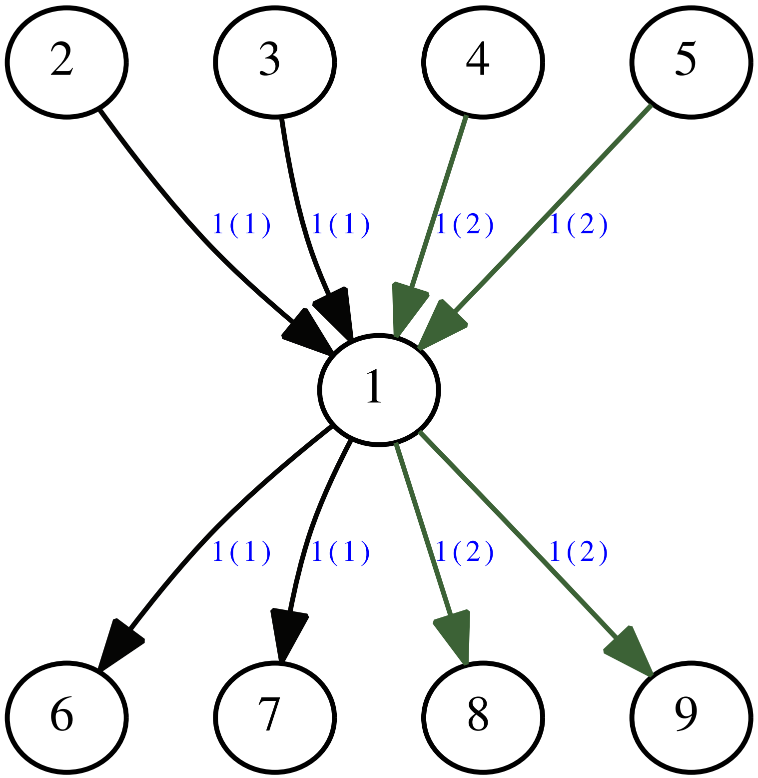

Feasible solution with 8 units of flow

Why is it unsustainable?

- Above solution is feasible
- Plant transforms one unit of **1,2** into 1 unit of **3** and 1 unit of **4**
- Input flow of 4 units of **1,2** produces eight units of **3,4**
- Only four units of **3,4** arrive at nodes 6,7,8,9
- **Four units wasted at plant**
- *We would like the model to warn us about this!*

Sustainability

“Sustainable”: working definition

Sustainable development:

a process network $G = (V, A)$ *where*

transformed flow is conserved

Forces to take into account every by-product of transformation process

Flow conservation

For $v \in V$ let $N^-(v) = \{u \in V \mid (u,v) \in A\}$ and $N^+(v) = \{u \in V \mid (v,u) \in A\}$

- *Conservation of* **ordinary flow** f:

$$\forall v \in V \qquad \sum_{u \in N^-(v)} f_{uv} - \sum_{u \in N^+(v)} f_{vu} = \omega_v$$

- *Conservation of* **multicommodity flow** f^k:

$$\forall v \in V, k \in K \qquad \sum_{u \in N^-(v)} f^k_{uv} - \sum_{u \in N^+(v)} f^k_{vu} = \omega^k_v$$

- *Conservation of* **transformation flow** *(*transflow*)* f^k:

$$\forall v \in V, k \in K \ \sum_{h \in K} \pi^{hk}_v \left(\omega^h_v + \sum_{u \in N^-(v)} f^h_{uv} \right) - \sum_{u \in N^+(v)} f^k_{vu} = \omega^k_v$$

Transflow properties

- No process can create something from nothing:

$$\forall v \in V, k \in K \quad \pi_v^{kk} \le 1$$

- No process cycle can create something from nothing:

$$\begin{aligned}\forall m \in \mathbb{N}, (k_i \mid i \le m) \in K^m, (v_i \mid i \le m) \in V^m \\ (v_1 = v_m \wedge \{(v_i, v_{i+1}) \mid i < m\} \subseteq A \quad \rightarrow \\ \pi_{v_1}^{k_1 k_2} \cdots \pi_{v_m}^{k_m k_1} \quad \le \quad 1)\end{aligned}$$

- Processes cannot destroy without transforming

$$\forall v \in V, k, h \in K \quad (\pi_v^{kh} \ge 0)$$

Transflow bounds

Taking into account budget and limit constraints

- **Limit constraints**: no process v can exceed its given transformation limit λ_v^k

$$\forall v \in V, k \in K \quad \omega_v^k + \sum_{u \in N^-(v)} f_{uv}^k \leq \lambda_v^k$$

- **Budget constraints**: transformation costs for commodity k at process node v are bounded above by budget B_v^k

$$\forall v \in V, k \in K \quad \gamma_v^k \left(\omega_v^k + \sum_{u \in N^-(v)} f_{uv}^k \right) \leq B_v^k$$

- Often consider aggregated versions of these constraints

Example

The simple transformation plant example yields an infeasible instance

```
presolve, variable f[2,1,2]:
impossible deduced bounds: lower = 0, upper = -2
presolve, variable f[4,1,1]:
impossible deduced bounds: lower = 0, upper = -2
presolve, variable f[4,1,1]:
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presolve, variable f[4,1,1]:
impossible deduced bounds: lower = 0, upper = -2
Infeasible constraints determined by presolve.
```

Model itself tells us it's wrong!

Percentages

A different interpretation

- $\pi_v^{hk} = 1, \pi_v^{h\ell} = 1$:

  1 unit of h is transformed into π_v^{hk} units of k and $\pi_v^{h\ell}$ units of ℓ

- **Example**: 1 coal $\longrightarrow$ 0.05 tar + 0.015 benzol + 500 methane
- Model inappropriate for some transformation processes
- **Example**: 50% of milk is pasteurised, 20% is transformed into cheese, 20% into butter and 10% is sold to other industries
- Decide percentages and flows to optimize process

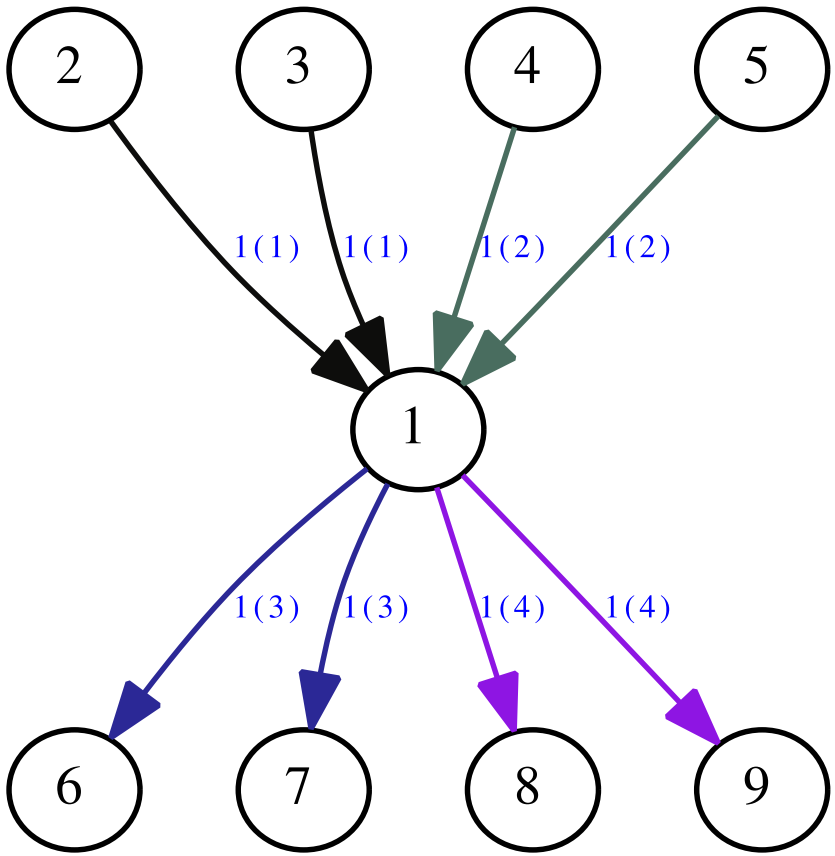
Formulation

- **Decision variables** p_v^{hk}: *percentage of h to be transformed into k at v*
- **Transflow conservation equations**:

$$\forall v \in V, k \in K \; \sum_{h \in K} \pi_v^{hk} p_v^{hk} \left(\omega_v^h + \sum_{u \in N^-(v)} f_{uv}^h \right) - \sum_{u \in N^+(v)} f_{vu}^k = \omega_v^k$$

- Interpretation : π no longer parameters but **decision variables**

Simple plant example



Solution: $p_1^{13} = p_1^{24} = 1$, $p_v^{14} = p_v^{23} = 0$

All **1** is transformed into **3**, all **2** into **4**: **sustainable**

Nonlinearity

- p, f, ω are decision variables
- Transflow conservation equations are bilinear (contain products $p\omega$, pf)
- Need a nonconvex NLP solver
- To find guaranteed global optima, need sBB (see PMA course)
- For example, COUENNE solver

Exact linearization 1

- **Exact linearization**: reformulation MINLP$\to$MILP s.t. GlobOpt$($MINLP$) =$ GlobOpt$($MILP$)$
- Aim: transform a nonconvex bilinear NLP into an LP
- Can use very efficient LP methods (simplex / interior point algorithm)
- In practice, can use CPLEX

Exact linearization 2

- Define new variables x (*quantity of commodity in process*)

$$\forall v \in V, k \in K \quad x_v^k = \omega_v^k + \sum_{u \in N^-(v)} f_{uv}^k$$

- Define new variables z (*q.ty of comm. to be transformed into another comm.*)

$$\forall v \in V, h, k \in K \quad z_v^{hk} = p_v^{hk} x_v^h \qquad (1)$$

- Linearization of Eq. (1): multiply $\forall v \in V, h \in H \ \sum_{k \in K} p_v^{hk} = 1$ by x_v^h, get

$$\forall v \in V, h \in H \quad \sum_{k \in K} z_v^{hk} = x_v^h$$

- Transflow conservation equations become:

$$\forall v \in V, k \in H \quad \sum_{h \in K} \pi_v^{hk} z_v^{hk} = \omega_v^k + \sum_{v \in N^+(v)} f_{uv}^k$$

Exact linearization 3

Thm.

The linearization is exact

Exact linearization 3

Thm.

The linearization is exact

Proof

Let (f', ω', x', z') be a solution of the LP. For all $v \in V, h, k \in K$ such that $x_v^h > 0$ we define $p_v^{hk} = \frac{z_v^{hk}}{x_v^h}$. If $x_v^h = 0$, we define $p_v^{hk} = 0$. In either case, the bilinear relation $z_v^{hk} = p_v^{hk} x_v^h$ is satisfied. This implies that the bilinear version of the transflow conservation equations hold.

Multiple input processes

Motivation

- Real transformation often require more types of input which transform as a whole
- **Example**: transformation of methane (mass only)

  $$1\ CH_4 + 2\ O_2 \longrightarrow 1\ CO_2 + 2\ H_2O$$

- π_v^{hk} makes no sense *(h, k should be sets of products)*
- Percentages p_v^{hk} are given
- Flow is **aggregated**

Multiple inputs

- A *multiple input transformation process* is a quadruplet $H = (H^-, H^+, p^-, p^+)$ with:
  - $H^-, H^+ \subseteq K$
  - $p^- : H^- \to \mathbb{R}_+$, $p^+ : H^+ \to \mathbb{R}_+$
- **Example**:
  - $H^- = \{\text{CH}_4, \text{O}_2\}$, $H^+ = \{\text{CO}_2, \text{H}_2\text{O}\}$
  - $p^- = (1, 2)$, $p^+ = (1, 2)$

Formulation

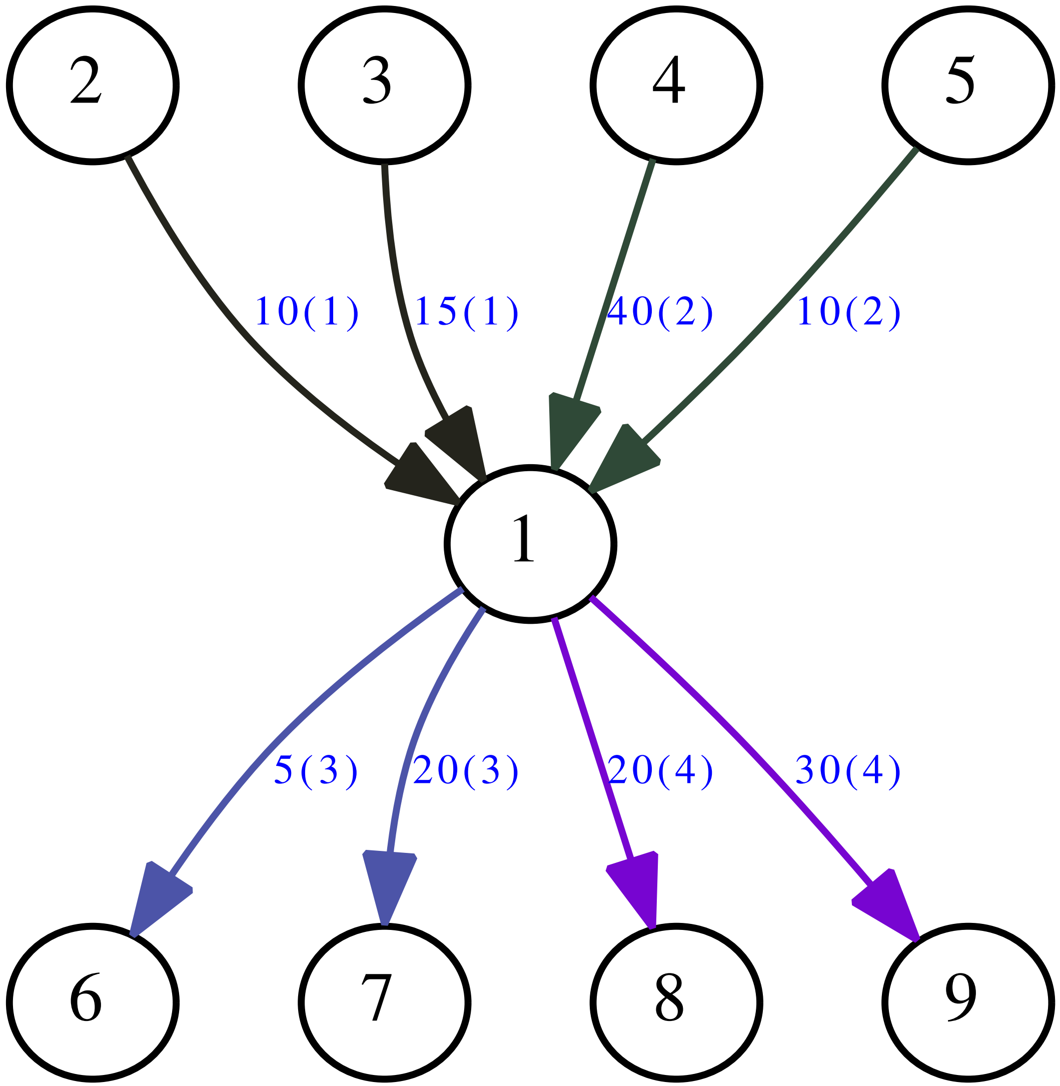
- Let:

$$\begin{aligned} x_v^k &= \omega_v^k + \sum_{u \in N^-(v)} f_{uv}^k \qquad \text{(inflow)} \\ y_v^k &= \omega_v^k + \sum_{u \in N^+(v)} f_{vu}^k \qquad \text{(outflow)} \end{aligned}$$

- *Multiple input transflow conservation*: let $H = (H^-, H^+, p^-, p^+)$,

$$\forall v \in V, H \in \mathcal{H}_v \qquad \sum_{k \in H^-} p_k^- x_v^k = \sum_{k \in H^+} p_k^+ y_v^k$$

Example



Chemical balances

Motivation

- Chemical reactions also produce **energy**
- Chemical formula:

  1 CH_4 + 2 O_2 $\longrightarrow$ 1 CO_2 + 2 H_2O + 891 kJ

- Equation

$$\mathsf{CH}_4 + 2\mathsf{O}_2 = \mathsf{CO}_2 + 2\mathsf{H}_2\mathsf{O} + 891\mathsf{kJ}$$

  makes no sense
- Can't mix molar equations with energy balances
- Think of **transformation engendering a new source of kJ** at plant node
- Can also engender a new target (absorption of energy)

Chemical transflows

- A *chemical transflow process* is a 8-tuplet $H = (H^-, H^+, p^-, p^+, J^-, J^+, q^-, q^+)$ with:
  - $H^-, H^+, J^-, J^+ \subseteq K$
  - $p^- : H^- \to \mathbb{R}_+$, $p^+ : H^+ \to \mathbb{R}_+$
  - $q^- : J^- \to \mathbb{R}_+$, $q^+ : J^+ \to \mathbb{R}_+$
  - $J^- \cap J^+ = \varnothing$
- **Example**:
  - $H^- = \{\mathsf{CH}_4, \mathsf{O}_2\}$, $H^+ = \{\mathsf{CO}_2, \mathsf{H}_2\mathsf{O}\}$
  - $J^- = \varnothing$, $J^+ = \{\mathsf{kJ}\}$
  - $p^- = (1, 2)$, $p^+ = (1, 2)$
  - $q^- = ()$, $q^+ = (891)$

New sources and targets

- Product $k \in J_v^+$ originates from a transformation at v
- Define a new source:

$$q_k^+ \omega_v^k = \sum_{u \in N^+(v)} f_{vu}^k$$

- Product $k \in J_v^-$ is absorbed by a transformation at v
- Define a new target:

$$q_k^- \omega_v^k = \sum_{u \in N^-(v)} f_{uv}^k$$

Ratios

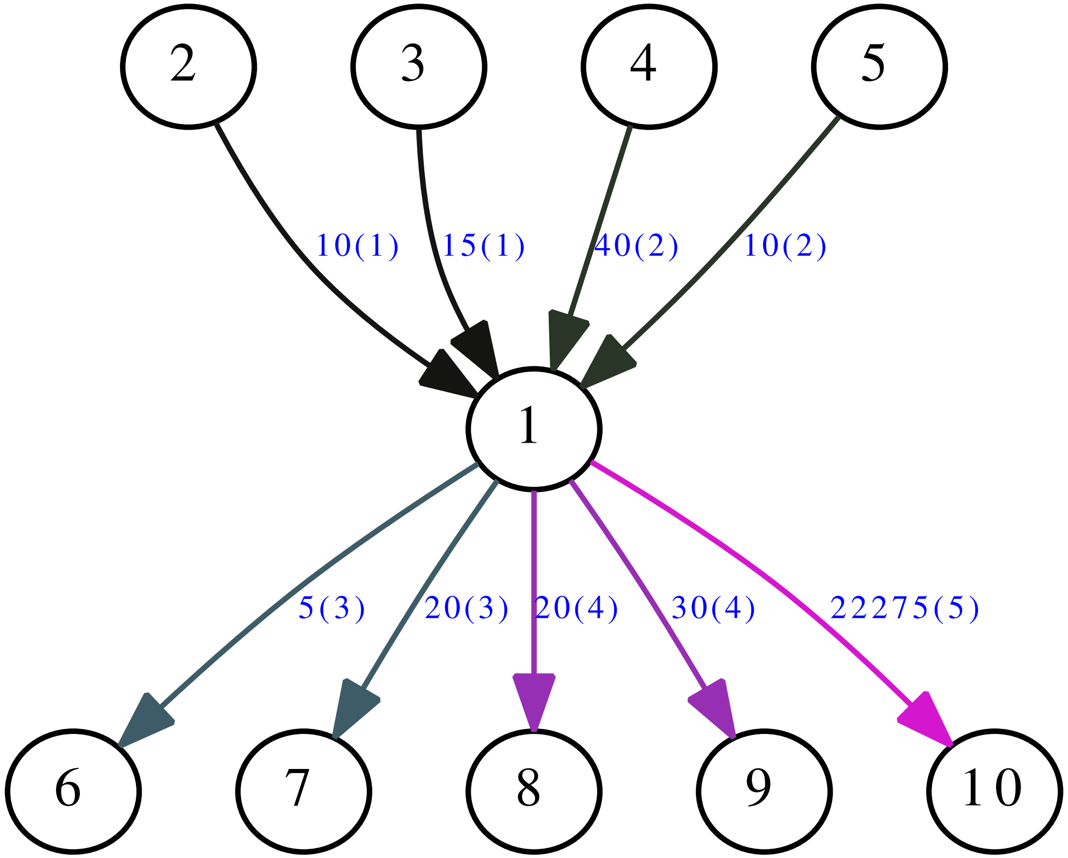
- $1\ CH_4 + 2\ O_2 \longrightarrow 1\ CO_2 + 2\ H_2O + 891\ \text{kJ}$ also implies:
  - $\frac{\text{oxygen}}{2} = \text{methane}$
  - $\text{carbon dioxide} = \text{methane}$
  - $\frac{\text{water}}{2} = \text{methane}$
  - $\frac{\text{energy}}{891} = \text{methane}$
- Enforce these as equations in the model

Formulation

- Let $H = (H^-, H^+, p^-, p^+, J^-, J^+, q^-, q^+)$, and $\bar{h} \in H^-$
- *Chemical transflow conservation*:

$$
\begin{array}{rrcl}
\forall v \in V, H \in \mathcal{H}_v & \sum_{k \in H^-} p_k^- x_v^k & = & \sum_{k \in H^+} p_k^+ y_v^k \\
\forall v \in V, H \in \mathcal{H}_v, k \in J^- & q_k^- \omega_v^k & = & \sum_{u \in N^-(v)} f_{uv}^k \\
\forall v \in V, H \in \mathcal{H}_v, k \in J^+ & q_k^+ \omega_v^k & = & \sum_{u \in N^+(v)} f_{vu}^k \\
\forall v \in V, H \in \mathcal{H}_v, k \in H^-(v) \smallsetminus \bar{h} & x_v^k / p_k^- & = & x_v^{\bar{h}} / p_{\bar{h}}^- \\
\forall v \in V, H \in \mathcal{H}_v, k \in H^+(v) & y_v^k / p_k^+ & = & x_v^{\bar{h}} / p_{\bar{h}}^- \\
\forall v \in V, H \in \mathcal{H}_v, k \in J^- & \omega_v^k & = & x_v^{\bar{h}} / p_{\bar{h}}^- \\
\forall v \in V, H \in \mathcal{H}_v, k \in J^+ & \omega_v^k & = & x_v^{\bar{h}} / p_{\bar{h}}^-
\end{array}
$$

Example



Near sustainability

Dealing with infeasibility

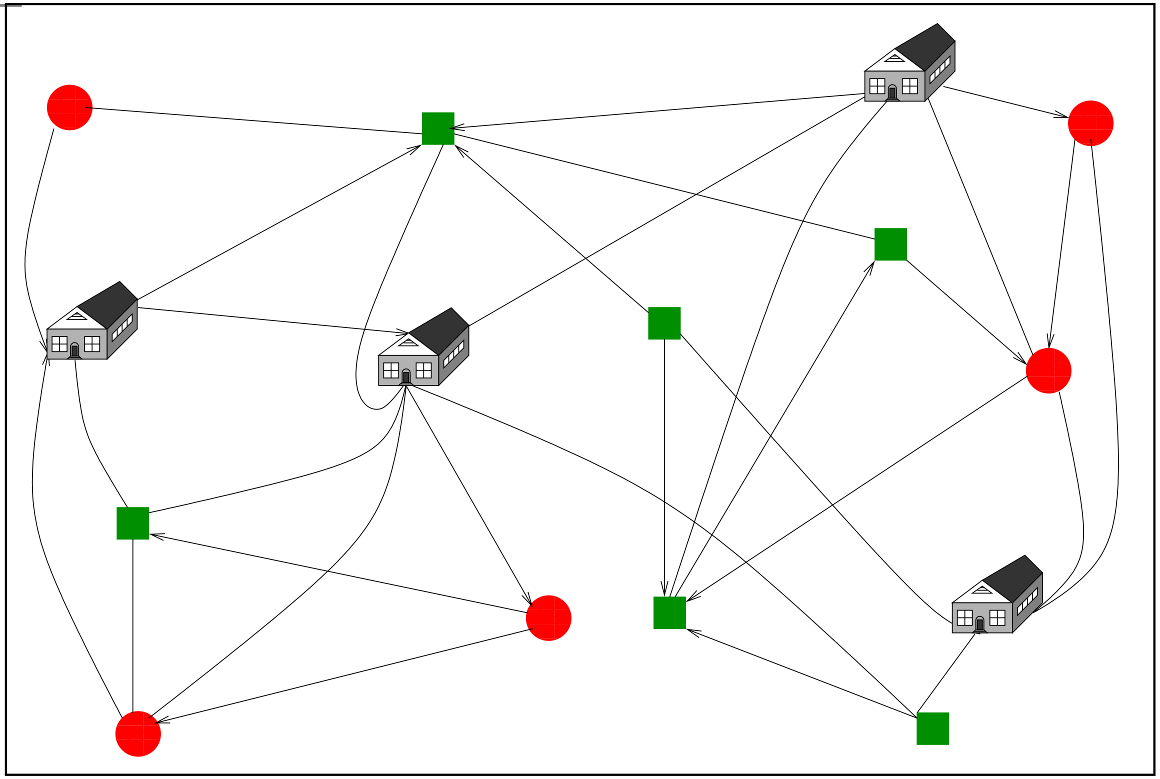
- Sometimes there is no feasible “purely sustainable” plan
- **Solution**: add bounded slacks to each equation

$$F(x) = 0 \qquad \longrightarrow \qquad F(x) = \epsilon_F$$
$$\epsilon_F^L \leq \epsilon_F \leq \epsilon_F^U$$

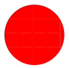
- ϵ is a decision variable
- Can also minimize:
  - $\sum_F \epsilon_F^2$,
  - $\sum_F |\epsilon_F|$,
  - $\max_F |\epsilon_F|$

Application to biomass production

Transform crops into energy



Route materials and energy optimally through this processing network

- : crop stocks (**provide raw materials to transform into energy)**
- : energy demand points (**processed energy must be routed to these points**)
- : transformation plants (**transform fixed proportions of materials into other materials/energy**)

A multi-commodity network

- Crops (■), demand points (●), plants (🏠) are all **nodes**
  V =set of nodes
- **Arcs** between nodes represent transportation lines
  A =set of arcs
- Materials and energy begin routed in the network are **commodities**
  H =set of commodities
- Other sets:
  - $H^-(v)$ =set of commodities that can enter node v
  - $H^+(v)$ =set of commodities that can exit node v
  - V_0 =set of nodes corresponding to plants

Node parameters

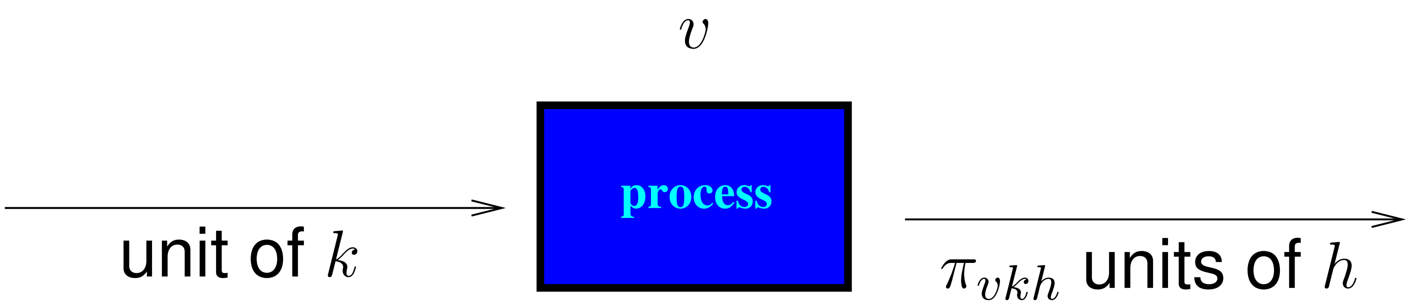
- c_{vk}: cost of supplying node v with a unit of commodity k
- C_{vk}: storage capacity for commodity k at node v
- d_{vk}: demand for commodity k at node v

Arc parameters

- τ_{uvk}: cost of transporting a unit of commodity k along arc (u, v)
- T_{uvk}: maximum amount of units of commodity k that can be transported across arc (u, v)

Transformation parameters

- λ_{vkh}: cost of transforming a unit of k into h at v
- π_{vkh}: quantity of h yielded per unit of k transformed at v



Decision variables

- x_{vk} =quantity of commodity k at vertex v
  $\forall v \in V, k \in H \quad d_{vk} \leq x_{vk} \leq C_{vk}$
- y_{uvk} =quantity of commodity k on arc (u, v)
  $\forall (u, v) \in A, k \in H \quad 0 \leq y_{uvk} \leq T_{uvk}$
- z_{vkh} =quantity of commodity k processed into commodity h at vertex v
  $\forall v \in V, k \in H^{-}(v), h \in H^{+}(v) \quad z_{vkh} \geq 0$
- For generality, all variables are indexed over all nodes, but not all apply (if not, fix them to 0)
  E.g. $x_{vk} = 0$ when $k \notin H^{-}(v) \cup H^{+}(v)$

Objective function

- Cost of supplying vertices with commodities:

$$\gamma_1 = \sum_{k \in H} \sum_{v \in V} c_{vk} x_{vk};$$

- Transportation costs:

$$\gamma_2 = \sum_{k \in H} \sum_{(u,v) \in A} \tau_{uvk} y_{uvk}$$

- Processing costs:

$$\gamma_3 = \sum_{v \in V} \sum_{k \in H^-(v)} \sum_{h \in H^+(v)} \lambda_{vkh} z_{vkh}$$

- **Objective function**: $\min \gamma_1 + \gamma_2 + \gamma_3$

Constraints

- **Composition of out-commodity**

$$\forall v \in V, h \in H^+(v) \qquad \sum_{k \in H^-(v)} \pi_{vkh} z_{vkh} = x_{vh}$$

- **In-commodity limit**

$$\forall v \in V, k \in H^-(v) \qquad \sum_{h \in H^+(v)} z_{vkh} \le x_{vk}$$

- **In- and out-commodity consistency**

$$\forall v \in V, k \in H^-(v) \qquad \sum_{(u,v) \in A} y_{uvk} \quad = \quad x_{vk}$$

$$\forall v \in V, h \in H^+(v) \qquad \sum_{(v,u) \in A} y_{vuh} \quad = \quad x_{vh}$$

Sustainable routing

- **Recycling**
  - Plants produce waste when processing
  - Waste from a given plant could be input to another type of plant
  - If this holds for every type of waste, we have a closed (sustainable) system
  - Also: negative cost $c_{vk} < 0$ where k is “waste”
    turning waste into energy derives profit from sales and servicing waste
- **Flow conservation**
  - Mass balance / flow conservation does not hold at plant nodes (i.e. those with $H^-(v) \neq H^+(v)$)

Planning the network construction

Network construction

- **Types of plant**: $P(v)$ =set of plant types that can be installed at node v
- **Parameters**:
  - λ_{vkhp} =cost of using plant $p \in P(v)$ to transform a unit of k into h at v
  - π_{vkhp} =yield of h using plant p as percentage of k at v
- **Decision variables**:

$$w_{vp} = \begin{cases} 1 & \text{if plant } p \text{ is installed at vertex } v \\ 0 & \text{otherwise} \end{cases}$$

- **Formulation changes**:
  - Replace λ_{vkh} by $\sum_{p \in P(v)} \lambda_{vkhp} w_{vp}$
  - Replace π_{vkh} by $\sum_{p \in P(v)} \pi_{vkhp} w_{vp}$

MINLP formulation

- **Processing costs**:

$$\gamma_3 = \sum_{v\in V} \sum_{k\in H^-(v)} \sum_{h\in H^+(v)} \left(\sum_{p\in P(v)} \lambda_{vkhp} w_{vp} \right) z_{vkh}$$

- **Composition of out-commodity**:

$$\forall v \in V, h \in H^+(v) \quad \sum_{k\in H^-(v)} \left(\sum_{p\in P(v)} \pi_{vkhp} w_{vp} \right) z_{vkh} = x_{vh}$$

- **Assignment consistency**:

$$\begin{array}{rccc} \forall v \in V_0 & \sum_{p\in P(v)} w_{vp} & \leq & 1 \\ \forall v \in V \setminus V_0 & \sum_{p\in P(v)} w_{vp} & = & 0 \end{array}$$

Citations

1. Bruglieri, Liberti, *Optimal running and planning of a biomass-based energy production process*, Energy Policy 2008
2. Bruglieri, Liberti, *Optimally running a biomass-based energy production process*, in Kallrath et al. (eds.), Optimization in the Energy Industry, 2009

The cost of risk equitability in hazardous material transportation

Transportation network

- Digraph $G = (V, A)$
- $\forall v \in V \quad N^+(v) = \{u \in V \mid (v, u) \in A\}$
- $\forall v \in V \quad N^-(v) = \{u \in V \mid (u, v) \in A\}$
- Arc weights:
  - $\ell : A \to \mathbb{R}_+$ (lengths, travelling time or traversal cost)
  - $C : A \to \mathbb{R}_+$ (arc capacity)

Commodities and zones

- *Commodities*:
  - Set $K = \{1, \ldots, K_{\text{max}}\}$ of commodity indices
  - Map $s : K \to V$ of source nodes for each commodity
  - Map $t : K \to V$ of target nodes for each commodity
  - Map $d : K \to \mathbb{R}$ of target demand for each commodity
- *Administrative zones*:
  - Set $Z = \{1, \ldots, Z_{\text{max}}\}$ of zones
  - Set $\zeta : Z \to \mathcal{P}(A)$ of arcs (routes) within each zone
    $\forall z \in Z \quad \zeta_z \subseteq A$

Damage and risk

- Map $p : A \to [0, 1]$: probability of accident on arc
- Map $\Delta : A \times K \to \mathbb{R}_+$: damage caused by accident with unit of commodity on arc
- For $(u, v) \in A, k \in K$: $r^k_{uv} = p_{uv}\Delta^k_{uv}$ is the *traditional risk*

Variables, objective

- *Decision variables*:
  - $x : A \times K \to \mathbb{R}_+$: flow of commodity on arc
- *Possible objective functions*:
  - **minimize total damage**:

$$\min \sum_{\substack{(u,v)\in A \\ k\in K}} \Delta_{uv}^k x_{uv}^k$$

  - **minimize total transportation cost**:

$$\min \sum_{\substack{(u,v)\in A \\ k\in K}} \ell_{uv} x_{uv}^k$$

  - Other objectives and linear combinations thereof

Basic constraints

- Arc capacity:

$$\forall (u,v) \in A \quad \sum_{k \in K} x^k_{uv} \leq C_{uv}$$

- Demand:

$$\forall k \in K \quad \sum_{v \in N^-(t_k)} x^k_{vt_k} = d_k$$

- Flow conservation:

$$\forall k \in K, v \in V \smallsetminus \{s_k, t_k\} \quad \sum_{u \in N^-(v)} x^k_{uv} = \sum_{u \in N^+(v)} x^k_{vu}$$

- **Also**: zero flow into sources and out of targets

Risk sharing constraints

- Risk sharing (*min pairwise risk difference*)

$$\forall z < w \in Z \quad \left| \sum_{\substack{(u,v)\in\zeta_z \\ k\in K}} r_{uv}^k x_{uv}^k - \sum_{\substack{(u,v)\in\zeta_w \\ k\in K}} r_{uv}^k x_{uv}^k \right| \leq R_D$$

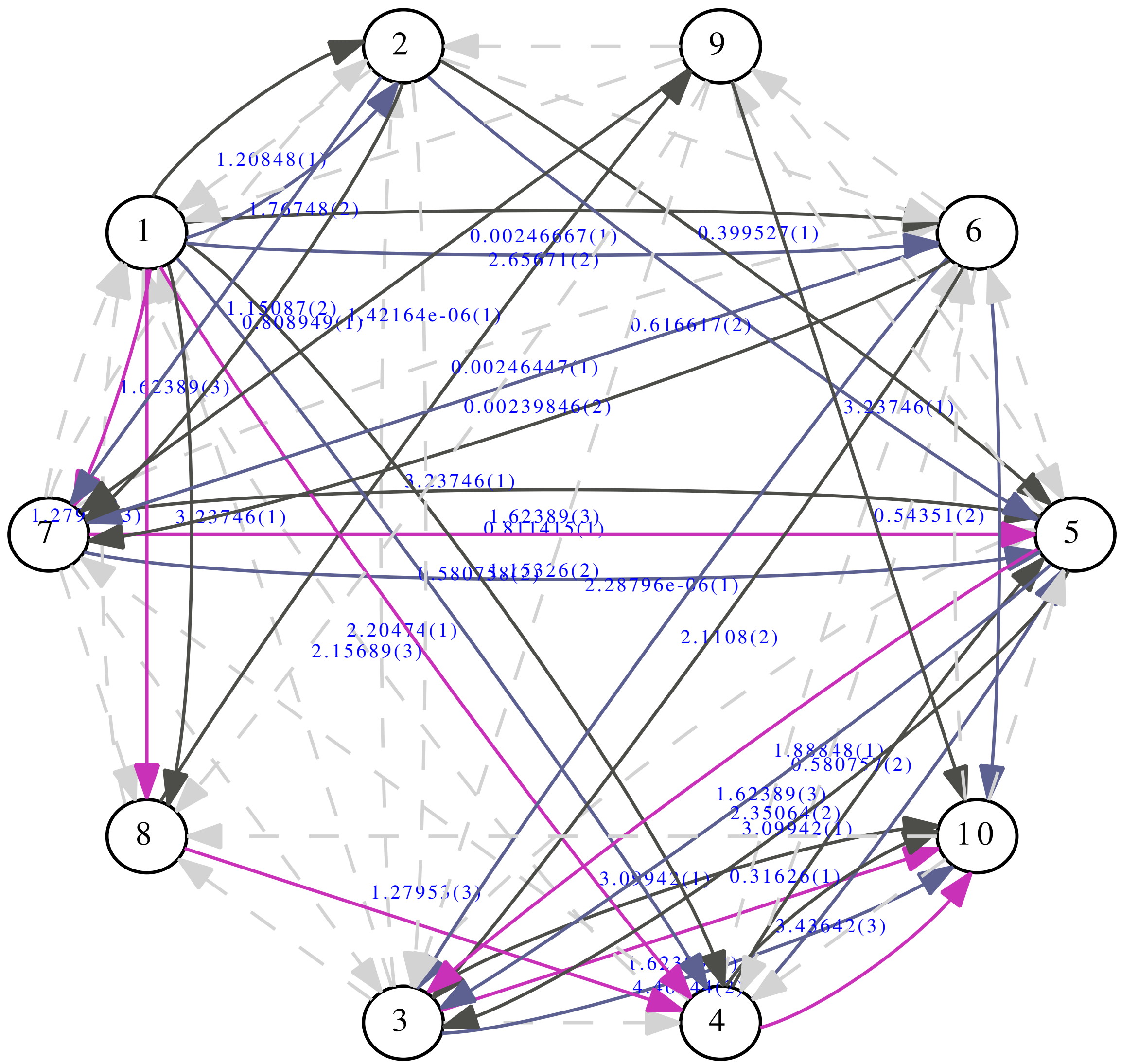
- Scalar R_D: inequitability threshold for risk sharing
- Rawls' principle (*min risk of riskiest zone*)

$$\forall z \in Z \quad \sum_{\substack{(u,v)\in\zeta_z \\ k\in K}} r_{uv}^k x_{uv}^k \leq R_P$$

- Scalar R_P: inequitability threshold for Rawls' principle

Random example 1

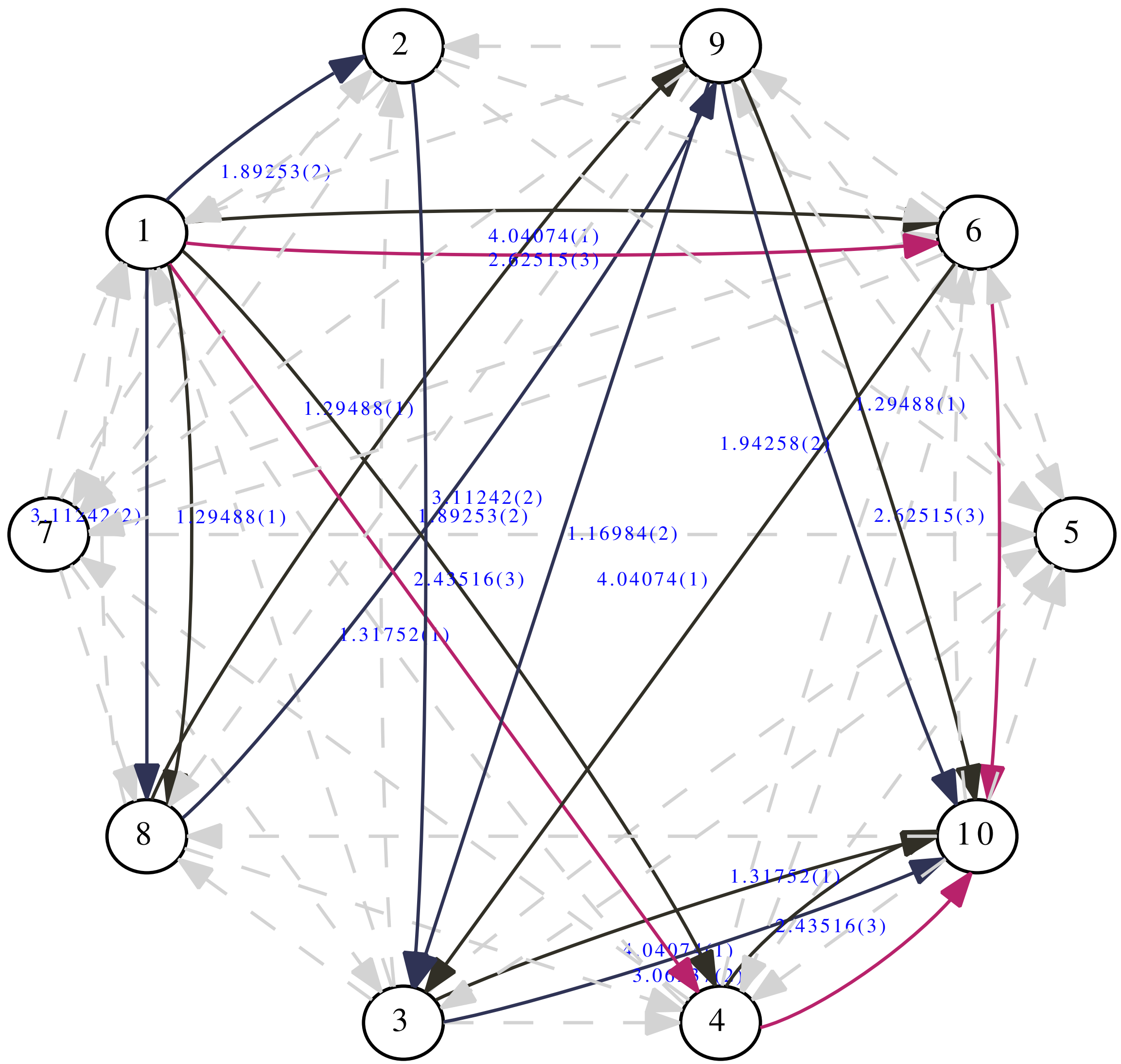
With risk sharing



$R_D = 10, R_P = 67.8$: total damage 855.045

Random example 1

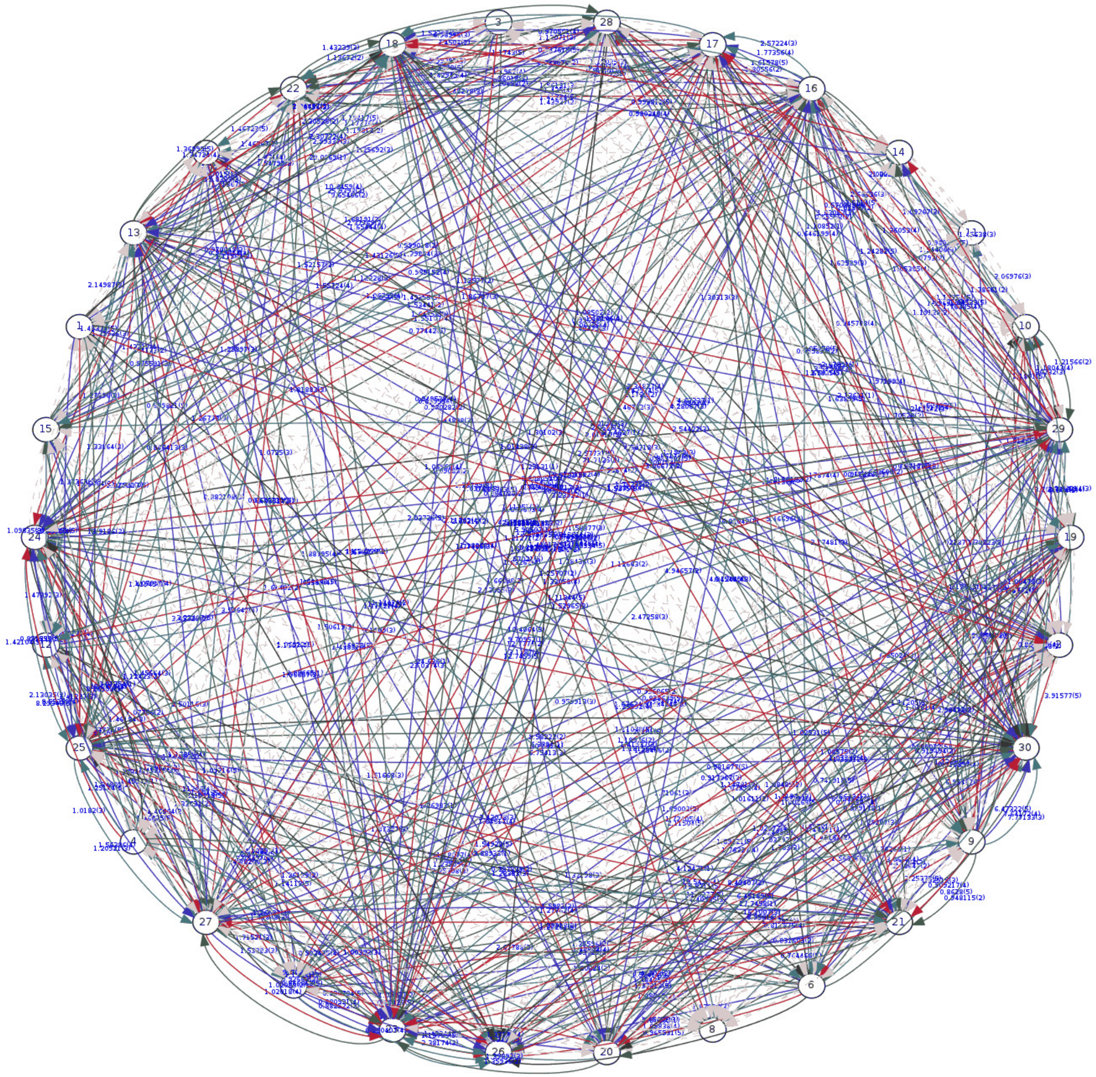
Without risk sharing



total damage 677.997 (< 855.045)

Random example 2

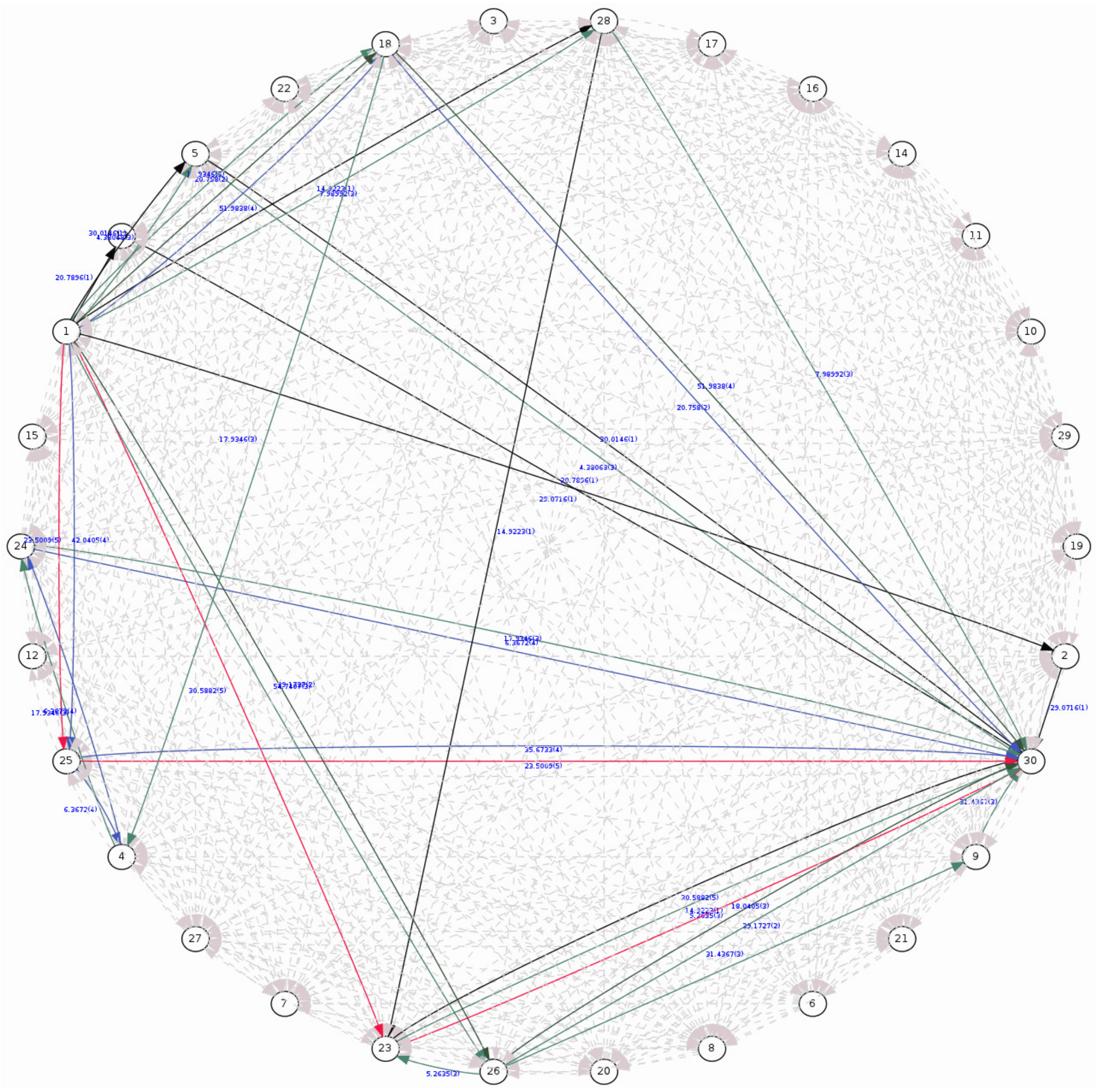
With risk sharing



$R_D = 10, R_P = 118.873$: total damage 38588

Random example 2

Without risk sharing



total damage 17647 (< 38588)

The moral of the story

Fairness has a cost

Announcement

Looking for smart PhD student for a thesis on *Smart buildings*
Funding provided by Microsoft Research
Co-directed by Y. Hamadi (MSR) and myself (LIX)
Requires optimization and simulation

The end