Port-Hamiltonian dynamics on graphs

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Contents

- The incidence matrix of a directed graph defines a Dirac structure, called the **vertex-edge Dirac structure**, which is used for defining port-Hamiltonian dynamics.
- Standard **consensus algorithms** are of this form, with **energy-storage** corresponding to the vertices and **energy-dissipation** corresponding to the edges.
- **Coordination control** is of this type, with energy storage **both at the vertices and on the edges**.
- By **Kirchhoff's current laws** another Dirac structure can be derived, called the **Kirchhoff-Dirac structure**. E.g. RLC-circuits are port-Hamiltonian with respect to the Kirchhoff-Dirac structure.
- **Chemical reaction networks**: from graphs to stochiometry.

General context and aim: providing a **modular** framework for **analyzing** and **synthesizing** large-scale systems:

- Component systems need to be interconnectable; need for **interconnection variables** and a clear 'interface'.
- Components can be re-used.
- Components can be independently refined and reduced/approximated.
- Dynamical properties to be inferred from dynamics of the components **and** the **interconnection structure**.
- Towards a synthesis theory of large-scale systems.

Preliminaries on **graphs**:

A **directed graph**, $\mathcal{G}$ is defined by a finite set $\mathcal{V}$ of **vertices** and a finite set $\mathcal{E}$ of directed **edges**, together with a mapping from $\mathcal{E}$ to the set of ordered pairs of $\mathcal{V}$., where no self-loops are allowed. Thus to any edge $e \in \mathcal{E}$ there corresponds an ordered pair $(v, w) \in \mathcal{V}^2$, with $v \neq w$, representing the initial vertex v and the final vertex w of this edge.

A directed graph, **graph** for short, is specified by its *incidence matrix* B, which is an $\bar{v} \times \bar{e}$ matrix, $\bar{v}$ being the number of vertices and $\bar{e}$ being the number of edges, with (i, j)-th element b_{ij} equal to 1 if the j-th edge is an edge towards vertex i, equal to -1 if the j-th edge is an edge originating from vertex i, and 0 otherwise.

Given a graph $\mathcal{G}$ we define its **vertex space** Λ_0 as the vector space of functions from $\mathcal{V}$ to $\mathbb{R}$, that is, $\mathbb{R}^{\bar{v}}$.

The **edge space** Λ_1 is the vector space of all functions from $\mathcal{E}$ to $\mathbb{R}$, that is $\mathbb{R}^{\bar{e}}$.

In the context of an **electrical circuit graph** Λ_1 is the vector space of currents through the edges in the circuit. The dual space of Λ_1 is denoted by Λ^1, and defines the vector space of voltages across the edges.

The duality product $< V|I >= V^T I$ of a vector of currents $I \in \Lambda_1$ with a vector of voltages $V \in \Lambda^1$ is the total power over the circuit. The dual space of Λ_0 is denoted by Λ^0 and defines the vector space of potentials at the vertices.

This can be extended by defining Λ_0, Λ_1, etc. as the vector space of functions from the vertices, resp. edges, to $\mathbb{R}^3$.

The incidence matrix B can be regarded as the matrix representation of a linear map (denoted by the same symbol)

$$B : \Lambda_1 \to \Lambda_0$$

called the **incidence operator**. Its adjoint map is denoted in matrix representation as

$$B^T : \Lambda^0 \to \Lambda^1,$$

and is called the **co-incidence** operator.

If we define Λ_0 and Λ_1 in the previous extended sense, then the incidence operator is given as

$$B \otimes I_3$$

A modular view on graphs

An **open graph** $\mathcal{G}$ is obtained from an ordinary graph by identifying a subset $\mathcal{V}_b \subset \mathcal{V}$ of **boundary vertices**.

$\mathcal{V}_b$ are the vertices that are open to interconnection (i.e., with other open graphs). The remaining subset $\mathcal{V}_i := \mathcal{V} - \mathcal{V}_b$ are the **internal vertices**.

Write correspondingly

$$\begin{aligned} \Lambda_0 &= \Lambda_i \oplus \Lambda_b \\ \Lambda^0 &= \Lambda^i \oplus \Lambda^b \end{aligned}$$

A subspace $\mathcal{D} \subset \mathcal{V} \times \mathcal{V}^*$ is a (constant) Dirac structure if

$$\mathcal{D} = \mathcal{D}^{\perp\!\!\!\perp}$$

where $^{\perp\!\!\!\perp}$ denotes the orthogonal complement with respect to the indefinite inner product $\ll \cdot, \cdot \gg$ on $\mathcal{V} \times \mathcal{V}^*$ defined as

$$\ll (v_1, v_1^*), (v_2, v_2^*) \gg := < v_1^* \mid v_2 > + < v_2^* \mid v_1 >,$$

with $v_1, v_2 \in \mathcal{V}, v_1^*, v_2^* \in \mathcal{V}^*$, where $< \cdot \mid \cdot >$ denotes the duality product between $\mathcal{V}$ and $\mathcal{V}^*$.

Example 1 *The graph of a skew-symmetric map from $\mathcal{V}$ to $\mathcal{V}^*$, or from $\mathcal{V}^*$ to $\mathcal{V}$ is Dirac structure.*
For any subspace $\mathcal{W} \subset \mathcal{V}$ the space $\mathcal{W} \times \mathcal{W}^\circ$ is a Dirac structure.

In the **finite-dimensional** case an equivalent characterization of Dirac structures is given as follows:

Proposition 2 *A subspace*

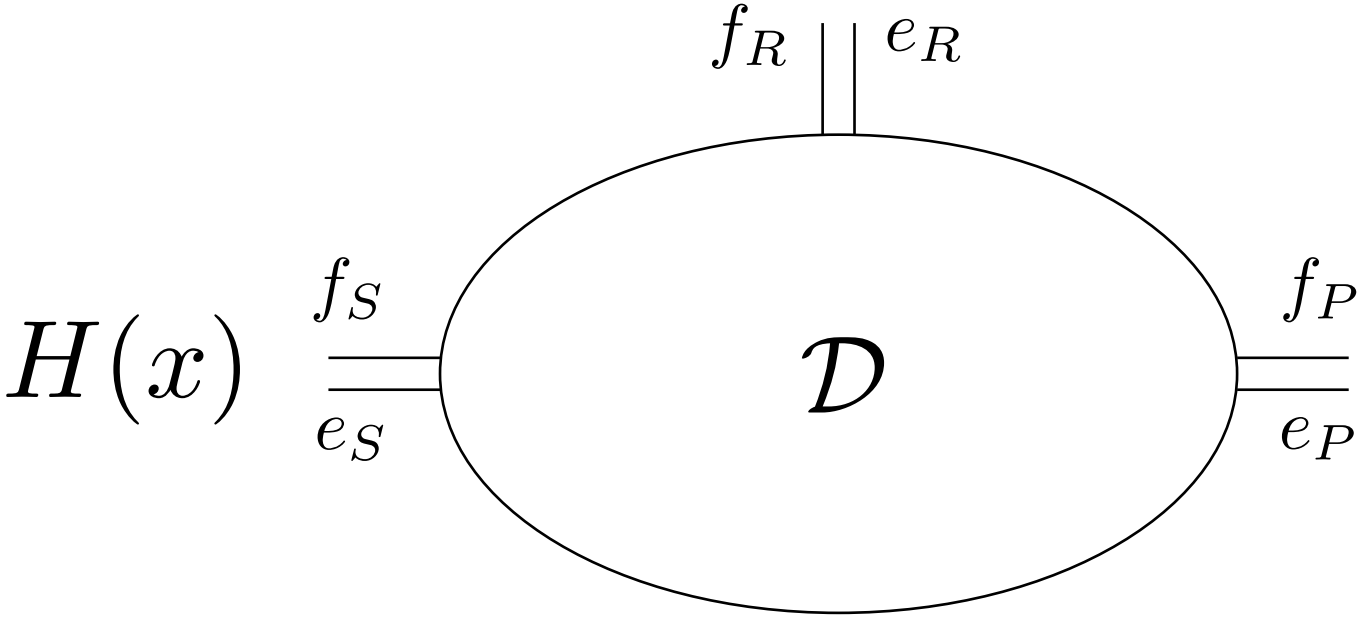
$$\mathcal{D} \subset \mathcal{V} \times \mathcal{V}^*$$

is a Dirac structure if and only if the following two conditions are satisfied:

$$\begin{aligned} &(i) < v^* \mid v >= 0, \qquad \textit{for all } (v, v^*) \in \mathcal{D} \\ &(ii) \dim \mathcal{D} = \dim \mathcal{V} \end{aligned} \tag{1}$$

Given a Dirac structure we can define **port-Hamiltonian systems**.

Geometric definition of a port-Hamiltonian system



The Hamiltonian $H : \mathcal{X} \to \mathbb{R}$ corresponds to energy-storage:

$$f_S = -\dot{x}, \quad e_S = \frac{\partial H}{\partial x}(x)$$

Furthermore, the resistive port is terminated by

$$R(f_R, e_R) = 0, \quad e_R^T f_R \leq 0$$

The vertex-edge Dirac structure on an open graph

Partition the incidence matrix B of an open graph as $B = \begin{bmatrix} B_i \\ B_b \end{bmatrix}$.

This defines the following Dirac structure, called the **vertex-edge Dirac structure**

$$\begin{aligned} \mathcal{D}_{ve}(\mathcal{G}) \quad := \quad & \{(f, e, f_i, e_i, f_b, e_b) \in \Lambda_1 \times \Lambda^1 \times \Lambda_i \times \Lambda^i \times \Lambda_b \times \Lambda^b \mid \\ & B_i f = -f_i, B_b f = -f_b, e = B_i^T e_i + B_b^T e_b\} \end{aligned}$$

This follows from

Proposition 3 *Let $A : \mathcal{V} \to \mathcal{W}$ be a linear map between the linear spaces $\mathcal{V}$ and $\mathcal{W}$, with adjoint mapping $A^* : \mathcal{W}^* \to \mathcal{V}^*$. Then*

$$\mathcal{D} := \{(v, w, v^*, w^*) \in \mathcal{V} \times \mathcal{W} \times \mathcal{V}^* \times \mathcal{W}^* \mid w = Av, v^* = -A^* w^*\}$$

is a Dirac structure.

Consensus algorithms as port-Hamiltonian systems

Assume the interaction topology of a network of agents is an **undirected graph** with set of edges $E(\mathcal{G})$ (symmetric interaction). The boundary vertices correspond to **leader** agents and the internal vertices to **follower** agents. Associate to each agent v a variable $x_v \in \mathbb{R}$ (or a vector $x_v \in \mathbb{R}^3$). A standard **consensus algorithm** is

$$\dot{x}_v(t) = - \sum_{(v,w)\in E(\mathcal{G})} g_{(v,w)}(x_v(t) - x_w(t))$$

for all **internal vertices** v, where $g_{(v,w)} > 0$ is a weight. Collecting all follower variables x_v into one vector x, and all leader variables x_v into u, endowing the graph with an arbitrary orientation, this is written

$$\dot{x} = -B_i G B_i^T x - B_i G B_b^T u$$

with B the incidence matrix, and G diagonal matrix with elements $g_e > 0$.

Hence in the absence of leader agents the consensus algorithm is

$$\dot{x} = -BGB^T x$$

For any incidence matrix B the matrix BB^T is known as the **graph Laplacian** matrix of the graph, and the matrix $L = BGB^T$ is called a **weighted** Laplacian matrix.

The graph Laplacian has many useful properties, characterizing, among others, the 'connectivity' of the graph.

Any symmetric positive semi-definite matrix L with diagonal elements ≥ 0, off-diagonal elements ≤ 0, and with zero row and column sums, can be written as a weighted Laplacian matrix $L = BGB^T$ of a certain graph, and conversely.

The consensus algorithm defines a **port-Hamiltonian system** with respect to the vertex-edge Dirac structure.

Indeed, the Hamiltonian function is simply given by

$$H(x) = \frac{1}{2} \parallel x \parallel^2$$

leading to the **energy storage** equations

$$\dot{x} = -f_i, \quad e_i = \frac{\partial H}{\partial x}(x) = x$$

Furthermore, the variables f, e correspond to the constitutive relations for **energy dissipation**

$$f = -Ge$$

The port-Hamiltonian system is explicitly given as

$$\begin{aligned} \dot{x} &= -B_i G B_i^T \frac{\partial H}{\partial x}(x) - B_i G B_b^T u \\ y &= B_b G B_i^T \frac{\partial H}{\partial x}(x) + B_b G B_b^T u \end{aligned}$$

with $u \in \Lambda^b$, $y = f_b \in \Lambda_b$, and $\frac{\partial H}{\partial x}(x) = x$.

We immediately obtain the energy balance

$$\frac{d}{dt} H = - \begin{bmatrix} x^T & u^T \end{bmatrix} B G B^T \begin{bmatrix} x \\ u \end{bmatrix} + y^T u$$

The consensus dynamics can be considered as the dynamics of unit masses (corresponding to each internal vertex), with linear dampers associated to the edges, and externally prescribed boundary velocities $u = e_b$ corresponding to the boundary vertices, and outputs $y = f_b$ being the boundary forces.

For a **connected** graph there exists for each vector $\bar{u}$ a unique equilibrium vector $\bar{x}$ such that

$$0 = -B_i G B_i^T \bar{x} - B_i G B_b^T \bar{u}$$

The function $f : \mathcal{V} \to \mathbb{R}$ defined as $f(v) = \bar{x}_v$ for each internal vertex v and $f(v_b) = \bar{u}_b$ for each boundary vertex v_b is called a **harmonic function**.

We obtain the following **shifted energy balance** property. Define the shifted Hamiltonian as

$$V(x) := H(x) - (x-\bar{x})^T \frac{\partial H}{\partial x}(\bar{x}) - H(\bar{x}) = \frac{1}{2}(x-\bar{x})^T(x-\bar{x})$$

Then

$$\frac{d}{dt}V(x) = -\begin{bmatrix}(x-\bar{x})^T & (u-\bar{u})^T\end{bmatrix} BGB^T \begin{bmatrix}x-\bar{x}\\ u-\bar{u}\end{bmatrix} + (y-\bar{y})^T(u-\bar{u})$$

where $\bar{y} = B_b G B_i^T \bar{x} + B_b G B_b^T \bar{u}$ is the output equilibrium value.

This shows (by LaSalle's Invariance principle) that for $u = \bar{u}$ the system converges to the maximal invariant set contained in

$$\{x \mid (x-\bar{x})^T B_i G B_i^T (x-\bar{x}) = 0\}$$

which (for a connected graph) is equal to the single point $\bar{x}$.
(Since for a connected graph $\ker BGB^T = \operatorname{span} \mathbb{1}$.)

Coordination control as a port-Hamiltonian system

Consider an open graph where each internal vertex corresponds to a port-Hamiltonin system. Coordination is achieved by designing a port-Hamiltonian dynamics associated to each edge.

Simplest case:

Let the dynamics associated to each internal **vertex** v be given by the integrator system

$$\begin{aligned} \dot{p}_v &= u_v \\ y_v &= \frac{\partial H_v}{\partial p_v}(p_v) \end{aligned}$$

These are coupled to the vertex-edge Dirac structure $\mathcal{D}_{ve}$ by setting

$$\begin{aligned} (u_1, \ldots, u_{\bar{v}}) &= -f_i \\ (y_1, \ldots, y_{\bar{v}}) &= e_i \end{aligned}$$

Design the port-Hamiltonian dynamics associated to each edge e as

$$\begin{aligned} \dot{q}_e &= w_e \\ z_e &= \frac{\partial H_e}{\partial q_e}(q_e) \end{aligned}$$

These are coupled to the vertex-edge Dirac structure $\mathcal{D}_{ve}$ by setting

$$\begin{aligned} (w_1, \ldots, w_{\bar{e}}) &= e \\ (z_1, \ldots, z_{\bar{e}}) &= -f \end{aligned}$$

The resulting system is given as the port-Hamiltonian system

$$\begin{aligned} \dot{q} &= B_i^T \frac{\partial H}{\partial p}(q,p) + B_b^T e_b \\ \dot{p} &= -B_i \frac{\partial H}{\partial q}(q,p) \\ f_b &= B_b^T \frac{\partial H}{\partial q}(q,p) \end{aligned}$$

where $q = (q_1, \ldots, q_{\bar{v}})$ and $p = (p_1, \ldots, p_{\bar{e}})$, and $H(q,p)$ denotes the total Hamiltonian.

In a typical formation control context, p_v is a **momentum** variable, and q_e is a **configuration** variable. Furthermore, e_b is an external (reference) **velocity** vector, and f_b the corresponding generalized **force** vector.
Thus the total system is a 'mass-spring system' with masses corresponding to the vertices and springs corresponding to the edges.

Asymptotic stability to the minimum of H will result if 'sufficient' damping is present either in the vertex or in the edge dynamics. For example, if the vertex dynamics is

$$\dot{p}_v = -K_v p_v + u_v, \qquad K_v > 0$$

Set-up can be easily extended by associating general port-Hamiltonian dynamics to each edge and each vertex.

Multi-machine power systems

$$\begin{aligned} \dot{\delta}_v &= \xi_v + \omega_s \\ M_v\dot{\xi}_v &= -K_v(M_v\xi_v) - \textstyle\sum_{w\neq v} E_v E_w B_{vw}[\sin(\delta_v - \delta_w) - \sin(\theta^*_{vw})] \end{aligned}$$

where δ_v is the angle of the rotor shaft, ω_s is the synchronous speed for the network, ξ_v is the deviation from this synchronous speed, and θ^*_{vw} is the equilibrium value for $\delta_v - \delta_w$.
In this case

$$H_v(p_v) = \frac{1}{2M_v}p_v^2$$

$$H_e(q_e) = E_i E_j B_{ij}[-\sin(q_e) + \cos(q_e^*) - \sin(\theta^*_{vw})(q_e - \theta^*_{vw})]$$

Kirchhoff-Dirac structure

Graphs and Kirchhoff's laws[a]

Figure 1: Kirchhoff

[a] G. Kirchhoff, *Über die Auflösung der Gleichungen, auf welche man bei der Untersuchung der Linearen Verteilung galvanische Ströme geführt wird*, Ann. Phys. Chem. 72, pp. 497–508, 1847.

Consider the **vertex-edge Dirac structure**

$$\mathcal{D}_{ve}(\mathcal{G}) := \{(f, e, f_i, e_i, f_b, e_b) \in \Lambda_1 \times \Lambda^1 \times \Lambda_i \times \Lambda^i \times \Lambda_b \times \Lambda^b \mid$$

$$B_i f = -f_i, B_b f = -f_b, e = B_i^T e_i + B_b^T e_b\}$$

and compose this Dirac structure with the trivial Dirac structure

$$\{(f_i, e_i) \mid f_i = 0\}$$

This yields the **Kirchhoff-Dirac structure**

$$\mathcal{D}_K(\mathcal{G}) := \{(f, e, f_b, e_b) \in \Lambda_1 \times \Lambda^1 \times \Lambda_b \times \Lambda^b \mid$$

$$B_i f = 0, \exists e_i \text{ s.t. } B_b f = -f_b, e = B_i^T e_i + B_b^T e_b\}$$

This is the Dirac structure underlying the modeling of e.g. RLC-circuits. The constraints $0 = -f_i = B_i f$ are **Kirchhoff's current laws** at the internal vertices. In this case, energy-dissipation and energy-storage are **both** associated to the **edges**.

Special case

The behavior of a purely resistive circuit at its terminals can be characterized by a linear input-output map

$$I_b = L_b \psi_b$$

where ψ_b are the potentials at the boundary vertices, and the matrix L_b has the properties of a weighted Laplacian matrix, that is

a symmetric positive semi-definite matrix with diagonal elements ≥ 0, off-diagonal elements ≤ 0, and with zero row and column sums

Open question: how to characterize the terminal behavior of RLC-circuits ?

Chemical reaction networks

Chemical reactions satisfy the **balance laws**

$$\dot{x} = Sv$$

where

$$x = (x_1, x_2, \cdots, x_n)^T$$

denotes the vector of **concentrations** (or mole numbers) of n chemical species, and

$$v = (v_1, v_2, \cdots, v_m)^T$$

denotes the vector of **fluxes** corresponding to m chemical reactions among these species.
The $n \times m$ matrix S is called the **stochiometric matrix**.

Example 4 *For example, the single chemical reaction*

$$A + 2B \to C$$

will have the stochiometric matrix (vector)

$$S = \begin{bmatrix} -1 \\ -2 \\ 1 \end{bmatrix}$$

A typical size of S of metabolic network of a cell is 540×609: large and with more reactions than species.

Furthermore, metabolic reaction networks involve **boundary** (exchange) fluxes v_b. This leads to a splitting of the stochiometric matrix as

$$\begin{bmatrix} S & S_b \end{bmatrix}$$

comparable to the splitting of the incidence matrix of a graph.

How to express v as a function of x ?

Basic option is **mass action kinetics**.

The reversible reaction

$$A + B \leftrightarrow C$$

is a combination of the **forward reaction**

$$A + B \rightarrow C$$

with rate equation $r_f = k_f ab$, and the **reverse reaction**

$$A + B \leftarrow C$$

with rate equation $r_r = k_r c$.

The net rate is thus the mass-action kinetics

$$v = r_f - r_r = k_f ab - k_r c$$

More generally, the reversible reaction

$$mA + nB \leftrightarrow pC + qD$$

has net reaction rate

$$v = k_f a^m b^n - k_r c^p d^q$$

A thermodynamical and port-Hamiltonian perspective

Consider the 'chemical reaction part' of Gibbs law

$$dG = \Sigma \mu_i(n) dn_i$$

with G the Gibbs free energy.
We would like to express the change in mole numbers $\dot{n}$ as a function of $\mu(n)$.
Or better, we want to express the flux variables v as functions of the vector of so-called **chemical affinities**

$$A = S^T \mu$$

(Note that $\mu(n)^T \dot{n} = A^T v$.) This will define the dynamics on $\mathbb{R}^m$, the space of reaction extents.
In general (far from thermodynamical equilibrium) this is **not** possible.

In case of e.g. mass action kinetics (and other cases) we can however do the following (see the work of Oster, Perelson and Katchalsky).
Write the stochiometric matrix S as $S = S_r - S_f$, where

S_f stochiometric matrix corresponding to reactants

S_r stochiometric matrix corresponding to products

Define the **forward** and **reverse** chemical affinities

$$\begin{bmatrix} A_f \\ A_r \end{bmatrix} = \begin{bmatrix} S_f^T \\ S_r^T \end{bmatrix} \mu = \begin{bmatrix} S_f & S_r \end{bmatrix}^T \mu$$

while we rewrite the mass balance equations as

$$\dot{x} = \begin{bmatrix} S_f & S_r \end{bmatrix} \begin{bmatrix} v_f \\ v_r \end{bmatrix}, \quad \begin{bmatrix} v_f \\ v_r \end{bmatrix} = \begin{bmatrix} -I \\ I \end{bmatrix} v$$

The dual relation is

$$A = \begin{bmatrix} -I & I \end{bmatrix} \begin{bmatrix} A_f \\ A_r \end{bmatrix} = -A_f + A_r = S^T \mu$$

Now the net rate equation is of the form

$$v = r_f(A_f) - r_r(A_r)$$

This leads to a port-Hamiltonian dynamics

$$\begin{aligned} \dot{n} &= S[r_f(A_f) - r_r(A_r)] + S_b v_b \\ A_b &= S_b^T \frac{\partial G}{\partial n} \end{aligned}$$

Conclusions

- On any directed (open) graph there is a canonical Dirac structure: the vertex-edge Dirac structure.
- Underlying consensus algorithms and coordination control strategies.
- Provides a 'physical' interpretation, and allows to unify results and employ techniques from Hamiltonian dynamics.
- Adding *Kirchhoff's current laws* at the internal vertices leads to the Kirchhoff-Dirac structure: merging graph theory with physical network dynamics.
- From the incidence matrix B to the stochiometric matrix S.

Port-Hamiltonian systems arsing from port-based network modeling

Port-based network modeling leads to a representation of a physical system as a **graph**, where each edge is decorated with a (vector) pair of **flow variables** $f \in \mathbb{R}^m$, and **effort variables** $e \in \mathbb{R}^m$, i.e., a **bond graph**

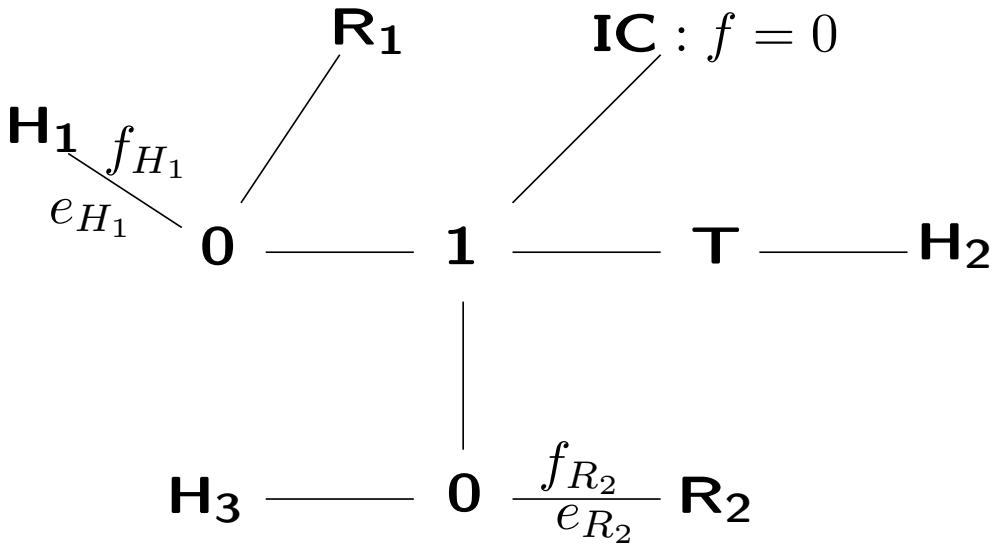


Figure 2: Port-based network modeling

and each vertex corresponds to one of the following *ideal elements*:

- *Energy-storing elements* H:

$$\begin{aligned} \dot{x} &= -f_H \\ e_H &= \frac{\partial H}{\partial x}(x), \quad H(x_1, \cdots, x_m) \in \mathbb{R} \text{ energy} \end{aligned}$$

- *Power-dissipating elements* R:

$$R(f_R, e_R) = 0, \quad e_R^T f_R \leq 0$$

- *Power-conserving elements*: transformers T, gyrators GY, ideal constraints IC.

- 0- *and* 1-*junctions*:

$$\begin{aligned} e_1 = e_2 = \cdots = e_k, \quad f_1 + f_2 + \cdots + f_k = 0 \\ f_1 = f_2 = \cdots = f_k, \quad e_1 + e_2 + \cdots + e_k = 0 \end{aligned}$$

- 0- and 1-junctions are the basic conservation laws of the system, and are also power-conserving:
  $e_1 f_1 + e_2 f_2 + \cdots + e_k f_k = 0$
- Transformers, gyrators are **energy-routing devices**, and may correspond to exchange between different types of energy.

All power-conserving elements have the following properties in common. They are described by **linear equations**:

$$F f + E e = 0, \quad f, e \in \mathbb{R}^l$$

whose solutions f, e satisfy

$$e^T f = e_1 f_1 + e_2 f_2 + \cdots + e_l f_l = 0,$$
$$\operatorname{rank} \begin{bmatrix} F & E \end{bmatrix} = l$$

All power-conserving elements taken together define a **Dirac structure**.