Introduction to bond graph theory

Second part: multiport field and junction structures, and thermodynamics

UNIVERSITAT POLITÈCNICA DE CATALUNYA

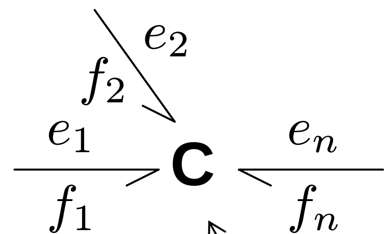
ACES
Advanced Control of Energy Systems

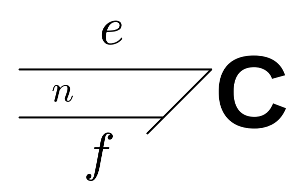
Multiport fields

We will look at multiport generalizations of C, I and R elements.

C-fields

Used mainly for sets of bonds with geometrical properties.





State variables $q_1, q_2, \ldots, q_n$

Allows easier displaying of individual causalities

$$\begin{aligned} \dot{q}_1 &= f_1 \\ \dot{q}_2 &= f_2 \\ &\vdots \\ \dot{q}_n &= f_n \end{aligned} \qquad \begin{aligned} e_1 &= \phi_1(q_1, \ldots, q_n) \\ e_2 &= \phi_2(q_1, \ldots, q_n) \\ &\vdots \\ e_n &= \phi_n(q_1, \ldots, q_n) \end{aligned}$$

Energy is computed as

$$H(t) = H(t_0) + \int_{t_0}^{t} \sum_{k=1}^{n} e_k(\tau) f_k(\tau) \, \mathrm{d}\tau$$

Changing $t \to q$ yields the line integral

$$H(q) = H(q_0) + \int_{\gamma} e(\tilde{q}) \, \mathrm{d}\tilde{q}$$

γ is any curve connecting q_0 and q

However, this must be independent of the particular curve connecting q_0 and q!

Barring topological obstructions, this is equivalent to

$$\frac{\partial \phi_i}{\partial q_j} = \frac{\partial \phi_j}{\partial q_i}, \quad i, j = 1, \dots, n$$

exactness of the 1-form given by e

$e = \mathrm{d}\phi$

Maxwell reciprocity condition

Linear case:

stiffness form

$$e = kq$$

all integral

compliance form

$$q = Ce$$

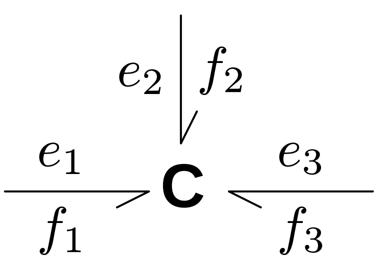
all differential

Mixed forms are also possible, but for a given system some of the forms, including the compliance one, may not exist.

The above nomenclature extends to the nonlinear case as well.

In the linear case, exactness of e implies that the matrices k and C, if the latter exists, are symmetric.

The available forms determine which causal patterns are admissible.

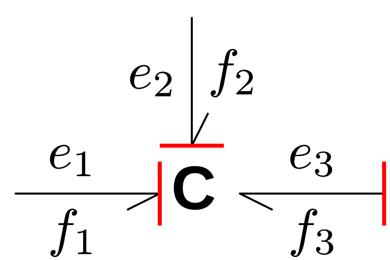


$$k = \begin{pmatrix} 2 & 0 & 2 \\ 0 & 1 & 1 \\ 2 & 1 & 3 \end{pmatrix}$$

$\det\ k = 0$ $\Longrightarrow$ all-integral is possible, all-differential is not

furthermore ...

$$\begin{pmatrix} q_1 \\ q_2 \\ e_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 & -1 \\ 0 & 1 & -1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ q_3 \end{pmatrix} \Longrightarrow$$

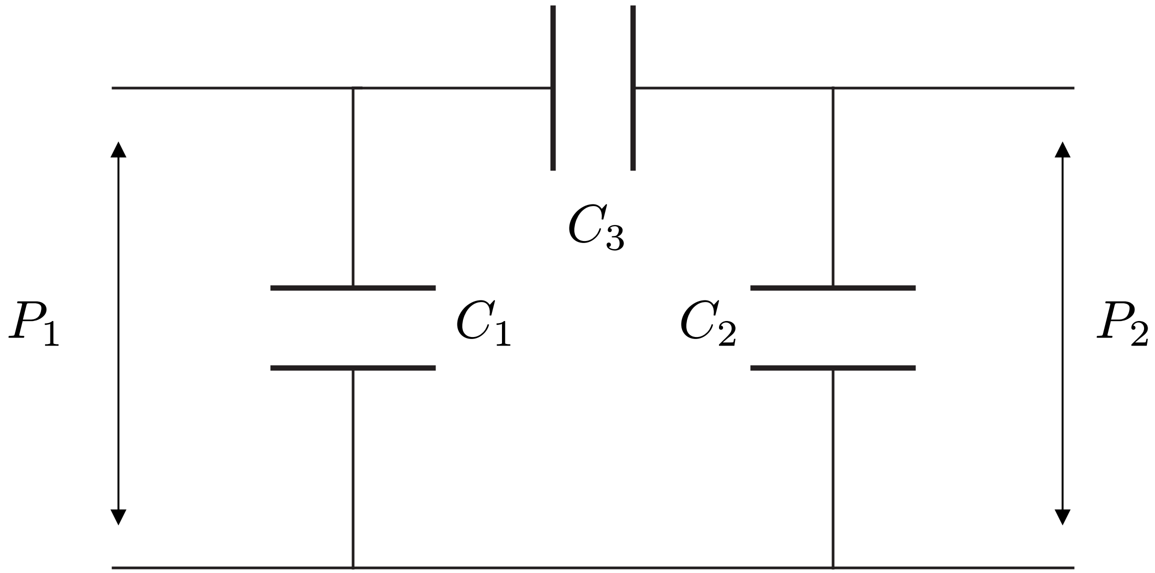


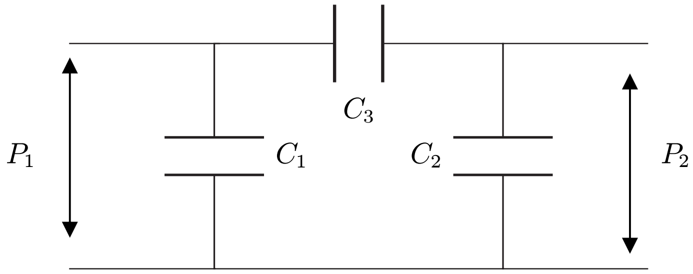
is possible

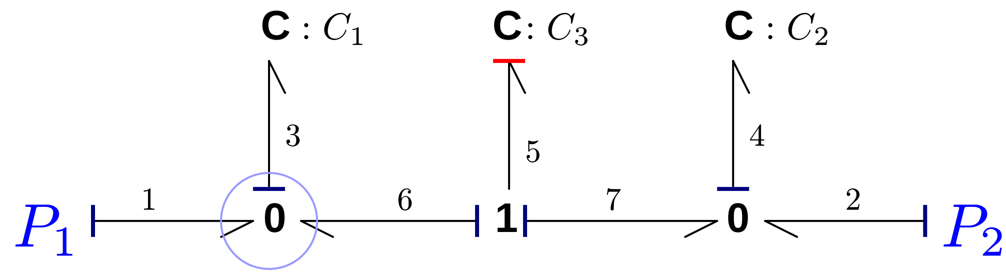
C-fields given from the beginning as a set of effort-displacement relations at n ports are called explicit.

Implicit C-fields are obtained when several C-elements are assembled by way of a power continuous network.

Implicit C-fields can be reduced to implicit form. In the process, some elements with differential causality may be hidden from the port interface.







$$e_1 = e_6 = e_3 \qquad f_6 = f_5 = f_7 \qquad e_4 = e_7 = e_2$$

$$f_3 = f_1 + f_6 \qquad e_5 = -e_6 - e_7 \qquad f_4 = f_7 + f_2$$

$$\dot{q}_3 = f_3 \qquad q_5 = C_3 e_5 \qquad \dot{q}_4 = f_4 \qquad f_1 = i_1$$

$$e_3 = \frac{1}{C_1} q_3 \qquad f_5 = \dot{q}_5 \qquad e_4 = \frac{1}{C_2} q_4 \qquad f_2 = i_2$$

$$q_5 = C_3 e_5 = C_3(-e_6 - e_7) = -C_3(e_3 + e_4) = -C_3 \left(\frac{q_3}{C_1} + \frac{q_4}{C_2} \right)$$

$$\dot{q}_5 = -C_3 \left(\frac{\dot{q}_3}{C_1} + \frac{\dot{q}_4}{C_2} \right)$$

$$\dot{q}_3 = f_3 = f_1 + f_6 = i_1 + f_5 = i_1 + \dot{q}_5 \; = i_1 - C_3\left(\frac{\dot{q}_3}{C_1} + \frac{\dot{q}_4}{C_2}\right)$$

$$\dot{q}_4 = f_4 = f_2 + f_7 = i_2 + f_5 = i_2 + \dot{q}_5 \; = i_2 - C_3\left(\frac{\dot{q}_3}{C_1} + \frac{\dot{q}_4}{C_2}\right)$$

$$\begin{pmatrix} 1 + \frac{C_3}{C_1} & \frac{C_3}{C_2} \\ \frac{C_3}{C_1} & 1 + \frac{C_3}{C_2} \end{pmatrix} \begin{pmatrix} \dot{q}_3 \\ \dot{q}_4 \end{pmatrix} = \begin{pmatrix} i_1 \\ i_2 \end{pmatrix}$$

$$\begin{pmatrix} \dot{q}_3 \\ \dot{q}_4 \end{pmatrix} = \frac{1}{C_1C_2 + C_2C_3 + C_1C_3} \begin{pmatrix} C_1C_2 + C_1C_3 & -C_1C_3 \\ -C_2C_3 & C_1C_2 + C_2C_3 \end{pmatrix} \begin{pmatrix} i_1 \\ i_2 \end{pmatrix}$$

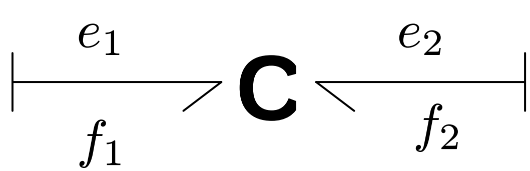
We introduce new state variables q_1, q_2 such that $\dot{q}_1 = i_1 = f_1$, $\dot{q}_2 = i_2 = f_2$.

Using $q_3 = C_1e_3 = C_1e_1$, $q_4 = C_2e_4 = C_2e_2$, and integrating in time:

$$\begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \frac{1}{C_1C_2 + C_2C_3 + C_1C_3} \begin{pmatrix} C_2 + C_3 & -C_3 \\ -C_3 & C_1 + C_3 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}$$

$$\begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \underbrace{\frac{1}{C_1C_2 + C_2C_3 + C_1C_3} \begin{pmatrix} C_2 + C_3 & -C_3 \\ -C_3 & C_1 + C_3 \end{pmatrix}}_{k} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}$$

This is a 2-port C-field in stiffness form.

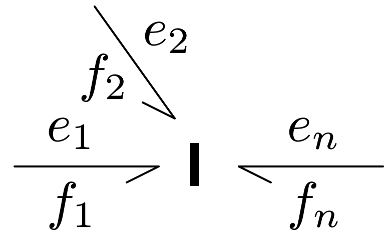


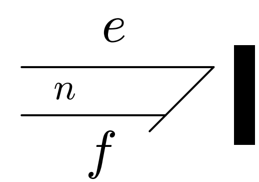
The state variables q_1, q_2 do not correspond to physical charges.

They are just a convenient parametrization of the $\mathbb{R}^3$ surface $q_5 = -C_3 \left(\frac{q_3}{C_1} + \frac{q_4}{C_2} \right)$

The dependent state variable has been hidden away from the port interface.

I-fields





State variables $p_1, p_2, \ldots, p_n$

$$\begin{array}{rclcrcl}
\dot{p}_1 & = & e_1 & \qquad & f_1 & = & \phi_1(p_1, \ldots, p_n) \\
\dot{p}_2 & = & e_2 & & f_2 & = & \phi_2(p_1, \ldots, p_n) \\
& \vdots & & & & \vdots & \\
\dot{p}_n & = & e_n & & f_n & = & \phi_n(p_1, \ldots, p_n)
\end{array}$$

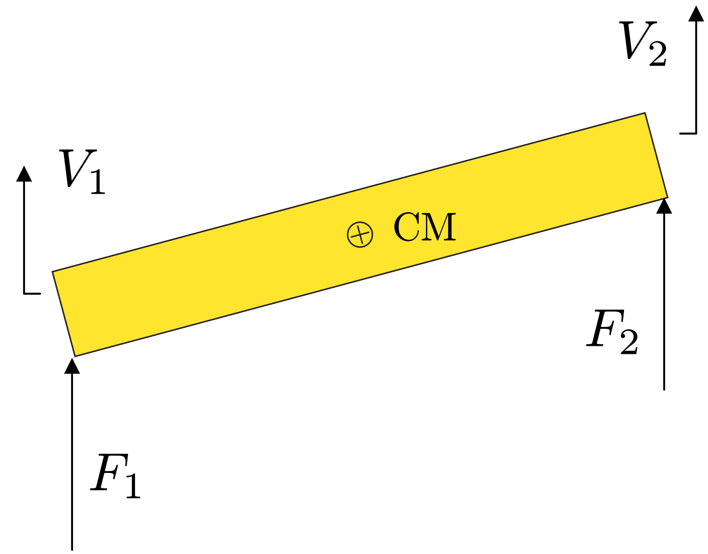
Energy:

$$H(p) = H(p_0) + \int_\gamma f(\tilde{p})\ \mathrm{d}\tilde{p} \qquad \frac{\partial \phi_i}{\partial p_j} = \frac{\partial \phi_j}{\partial p_i}, \quad i, j = 1, \ldots, n$$

independence of γ

Rigid bar with mass m, length L and moment of inertia J respect to the CM.

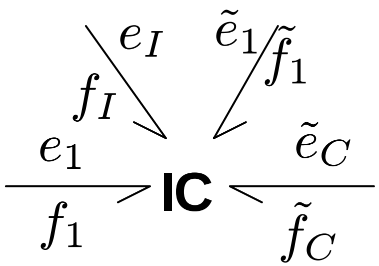
We consider only vertical displacements and small rotations around CM.



Under these assumptions, this can be described as an explicit I-field, with constitutive relation

$$\begin{pmatrix} V_1 \\ V_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{m} + \frac{L^2}{4J} & \frac{1}{m} - \frac{L^2}{4J} \\ \frac{1}{m} - \frac{L^2}{4J} & \frac{1}{m} + \frac{L^2}{4J} \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}$$

IC-fields



$$
\begin{aligned}
\dot{p}_1 &= e_1 & f_1 &= \phi_1(p_1, \ldots, p_I, q_1, \ldots, q_C) \\
&\vdots & &\vdots \\
\dot{p}_I &= e_I & f_I &= \phi_I(p_1, \ldots, p_I, q_1, \ldots, q_C) \\
\dot{q}_1 &= \tilde{f}_1 & \tilde{e}_1 &= \tilde{\phi}_1(p_1, \ldots, p_I, q_1, \ldots, q_C) \\
&\vdots & &\vdots \\
\dot{q}_C &= \tilde{f}_C & \tilde{e}_C &= \tilde{\phi}_I(p_1, \ldots, p_I, q_1, \ldots, q_C)
\end{aligned}
$$

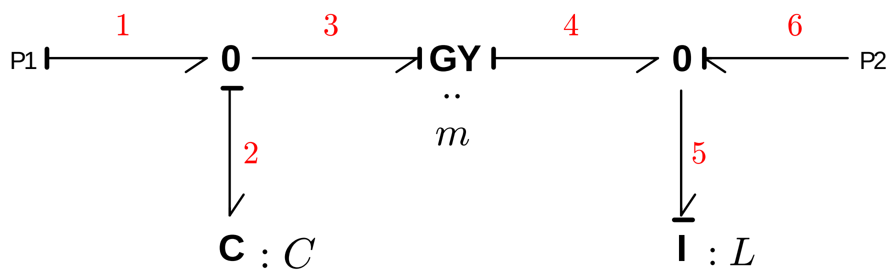
Maxwell reciprocity equations

$$
\frac{\partial \phi_i}{\partial p_j} = \frac{\partial \phi_j}{\partial p_i}, \quad i, j = 1, \ldots, I \qquad \frac{\partial \tilde{\phi}_i}{\partial q_j} = \frac{\partial \tilde{\phi}_j}{\partial q_i}, \quad i, j = 1, \ldots, C
$$

$$
\boxed{\frac{\partial \phi_i}{\partial q_j} = \frac{\partial \tilde{\phi}_j}{\partial p_i}, \quad i = 1, \ldots, I, \;\; j = 1, \ldots, C}
$$

A typical example of an IC-field is an **electrical solenoid** transducer.

A more academic example is



$$\begin{aligned} \dot{q}_2 &= f_1 - \frac{1}{m} e_6 \\ \dot{p}_5 &= e_6 \end{aligned}$$

To get an explicit IC-field, define state variables q, p such that $f_1 = \dot{q}$, $e_6 = \dot{p}$

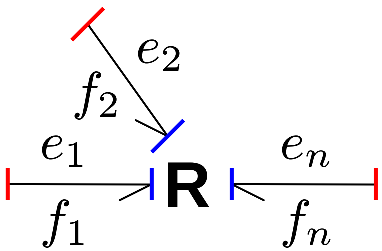
$p = p_5$, $q = q_2 + \frac{1}{m} p_5$

$$\begin{aligned} e_1 &= \frac{1}{C} q - \frac{1}{mC} p \\ f_6 &= -\frac{1}{mC} q + \left(\frac{1}{L} + \frac{1}{m^2 C} \right) p \end{aligned}$$

Maxwell condition

R-fields

Onsager forms



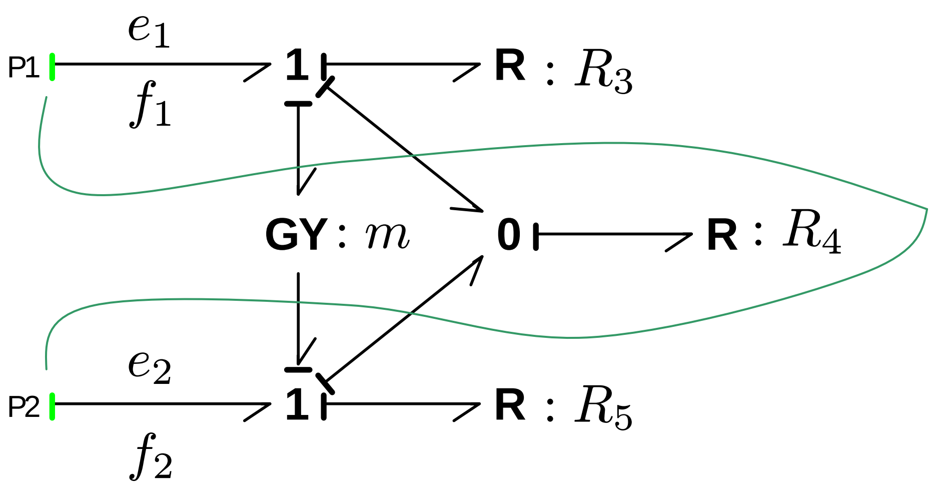
resistance form $\quad e = \Phi(f)$

conductance form $\quad f = \Phi^{-1}(e)$

Mixed causality forms may also be possible

In the linear case, implicit R-fields without gyrators or sources have Onsager forms with symmetric matrices.

If some (e, f) pairs are interchanged in their causality from an Onsager form, the corresponding matrix adquires antisymmetric terms. Such contitutive relations are said to be in Casimir form.



Several forms are possible by switching the causality around.

$$\begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} R_3 + R_4 & m + R_4 \\ -m + R_4 & R_4 + R_5 \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

This Onsager form is not symmetric, due to the presence of a gyrator.

Junction structures

Assemblages of 0, 1, TF and GY elements which switch energy around.

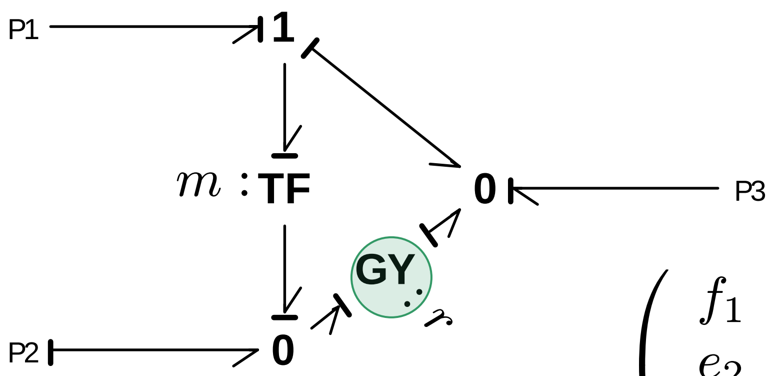
Limiting cases of R-fields (without sources)which do not dissipate.

Unless modulated TF or GY elements are present, effort/flow constitutive relations in a junction structure are always linear.

With an all-input power sign convention, the matrix relating inputs to outputs must be antisymmetric.

Causality patterns are more restricted, though.

Junction structures without gyrators cannot accept conductance or resistance causality on all ports.

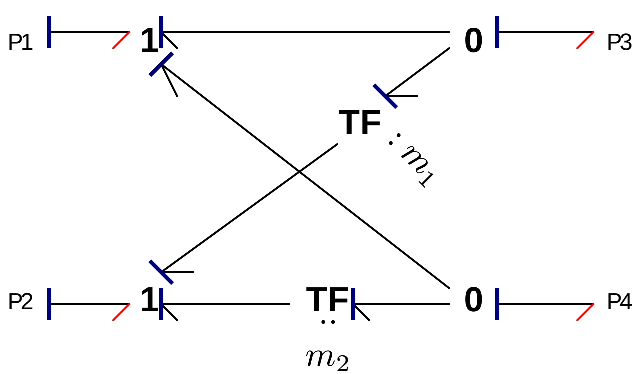


Pure conductance or resistance forms are not possible.

$$\begin{pmatrix} f_1 \\ e_2 \\ f_3 \end{pmatrix} = \begin{pmatrix} 0 & -m & \frac{m}{r} \\ m & 0 & -m \\ -\frac{m}{r} & m & 0 \end{pmatrix} \begin{pmatrix} e_1 \\ f_2 \\ e_3 \end{pmatrix}$$

Multiport transformers are an special case of junction structures.

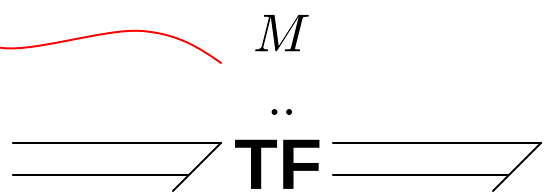
Through-power convention



With an all-input power convention, (e_1, e_2, f_3, f_4) would be obtained from (f_1, f_2, e_3, e_4) with an antisymmetric matrix.

With the through-power convention, the matrix is symmetric and can be decomposed into two matrices wich are transpose:

$$\begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \boxed{\begin{pmatrix} 1 & 1 \\ m_1 & m_2 \end{pmatrix}} \begin{pmatrix} e_3 \\ e_4 \end{pmatrix} \qquad \begin{pmatrix} f_3 \\ f_4 \end{pmatrix} = \boxed{\begin{pmatrix} 1 & m_1 \\ 1 & m_2 \end{pmatrix}} \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$



The fact that the flow transformation is given by M^T ensures the power continuity.

Multiport transformers need not have the same number of inputs ans outputs.

Example: $abc \rightarrow dq$ transformation in induction machines.

Junction structures are also necessary to connect the bond graph formalism with port Hamiltonian and Dirac structure concepts.

Thermodynamics from the bond graph point of view

Pure substance with no motion, constant mass and
no electromagnetic or surface-tension forces:

$$u = u(s, v)$$

internal energy per unit mass

entropy per unit mass

volume per unit mass

Gibbs equation:

$$\mathrm{d}u = \boxed{T}\,\mathrm{d}s - \boxed{p}\,\mathrm{d}v$$

absolute temperature

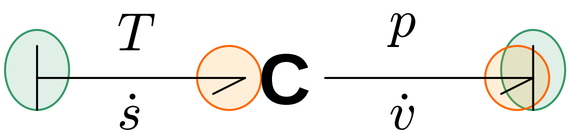
pressure

$$\mathrm{d}u = T\,\mathrm{d}s - p\,\mathrm{d}v \quad\Longrightarrow\quad \begin{cases} T = \dfrac{\partial u}{\partial s} \\[2ex] -p = \dfrac{\partial u}{\partial v} \end{cases} \quad\Longrightarrow\quad \frac{\partial T}{\partial v} = \frac{\partial(-p)}{\partial s}$$

Maxwell relation for a 2-port C-field with a power-through convention

T and p are efforts

$$\left.\begin{aligned} T &= T(s, v) \\ p &= p(s, v) \end{aligned}\right\} \text{ constitutive equations} \quad\Longrightarrow\quad \boxed{\text{for all-integral causality}}$$



$\dot{s}$ and $\dot{v}$ are the corresponding flows

In thermodynamics, mixed and all-derivative causality is implemented by means of Legendre transformations.

entalphy h

Gibbs equation

$$h = u + pv \quad \Longrightarrow \quad \mathrm{d}h = \mathrm{d}u + p\ \mathrm{d}v + v\ \mathrm{d}p = \boxed{T\ \mathrm{d}s + v\ \mathrm{d}p}$$

$$\Longrightarrow \quad h = h(s,p)$$

constitutive equations

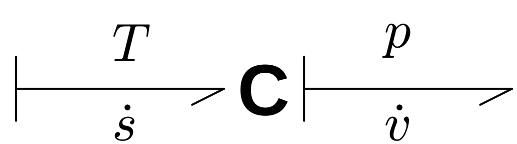
$$\begin{aligned} T &= T(s,p) \\ v &= v(s,p) \end{aligned}$$

$$\begin{aligned} T &= \frac{\partial h}{\partial s} \\ v &= \frac{\partial h}{\partial p} \end{aligned} \quad \Longrightarrow$$

Maxwell condition

$$\frac{\partial T}{\partial p} = \frac{\partial v}{\partial s}$$

mixed causality



Helmholtz free energy f

Gibbs equation

$$f = u - Ts \Longrightarrow \mathrm{d}f = \mathrm{d}u - T\,\mathrm{d}s - s\,\mathrm{d}T = \boxed{-s\,\mathrm{d}T - p\,\mathrm{d}v}$$

$$\Longrightarrow \quad f = f(T, v)$$

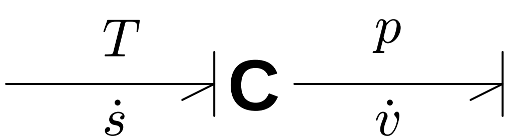
constitutive equations

$$\begin{aligned} s &= s(T, v) \\ p &= p(T, v) \end{aligned}$$

$$\begin{aligned} -s &= \frac{\partial f}{\partial T} \\ -p &= \frac{\partial f}{\partial v} \end{aligned} \Longrightarrow \quad \frac{\partial p}{\partial T} = \frac{\partial s}{\partial v}$$

Maxwell condition

mixed causality



Gibbs free energy ϕ

$$\phi = u + pv - Ts \Longrightarrow \mathrm{d}\phi = \mathrm{d}u + p\ \mathrm{d}v + v\ \mathrm{d}p - T\ \mathrm{d}s - s\ \mathrm{d}T$$

$$= \boxed{-s\ \mathrm{d}T + v\ \mathrm{d}p} \Longrightarrow \phi = \phi(T, p)$$

Gibbs equation

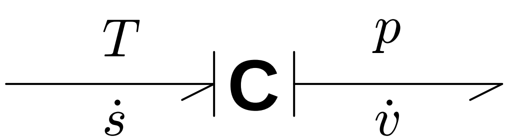
constitutive equations

$$\begin{aligned} s &= s(T,p) \\ v &= v(T,p) \end{aligned}$$

$$\begin{aligned} -s &= \frac{\partial \phi}{\partial T} \\ v &= \frac{\partial \phi}{\partial p} \end{aligned} \Longrightarrow \frac{\partial v}{\partial T} = \frac{\partial(-s)}{\partial p}$$

Maxwell condition

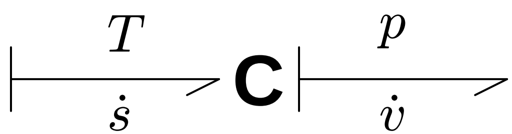
All-differential causality

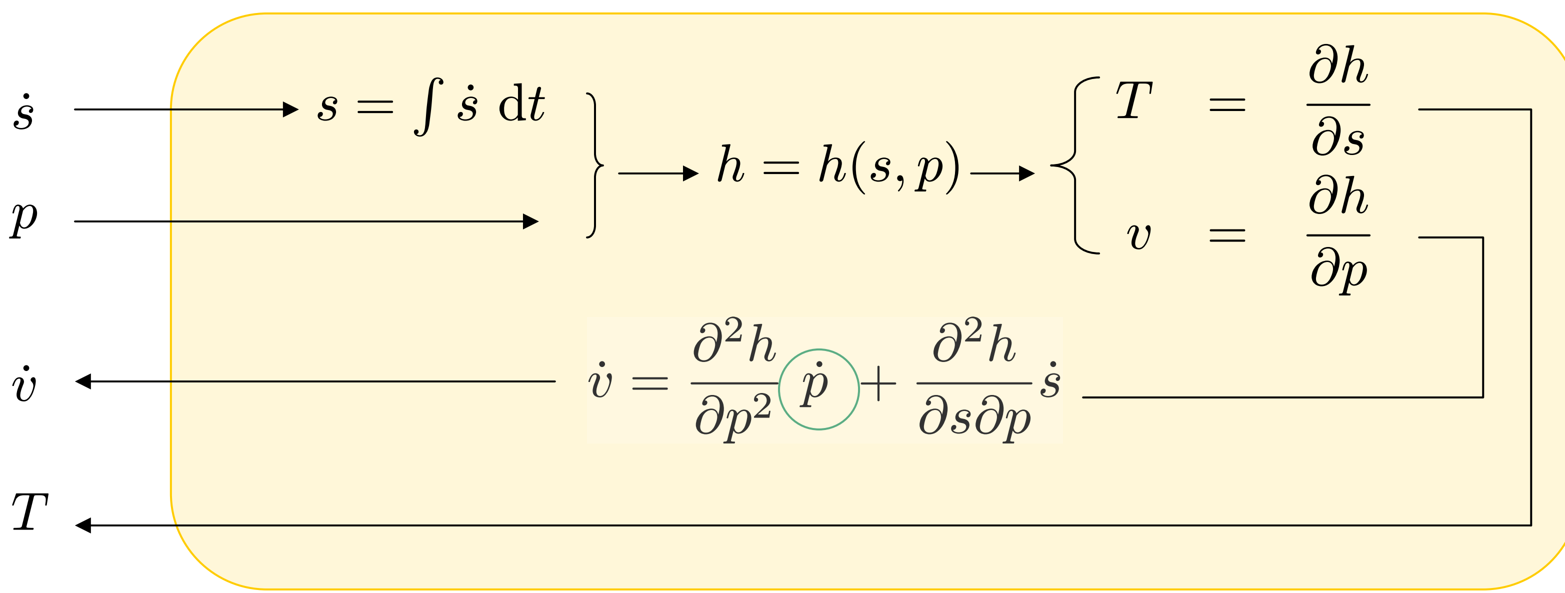


Any of the four formulations gives constitutive equations which guarantee conservation of energy.

The computation path depends on the causality pattern.

For instance, assume the entalphy is given, $h = h(s, p)$





One can also give constitutive equations without using any of the energy functions u, h, f or ϕ.

However, this can easily give *impossible* substances, which violate the First Principle of Thermodynamics (energy conservation).

Ideal gas:

$$pv = RT$$

Since this is a pure substance of the type considered, another constitutive equation is needed to specify the 2-port.

The remaining equation is related to the gas being mono- or diatomic.

Giving this second equation arbitrarily runs into the above problem.

It is better to start with two other relations and build an energy function from them, incorporating $pv = RT$.

specific heat at constant pressure

$$c_p = \frac{\partial h}{\partial T}$$

this makes sense since p is an input in the $h(s,p)$ formulation

T is not a natural variable of h or u.

specific heat at constant volume

$$c_v = \frac{\partial u}{\partial T}$$

this makes sense since $\dot{v}$ is an input in the $u(s,v)$ formulation

Together with $pv = RT$, we assume that c_v is a constant, determined by the particular ideal gas.

$$\left.\begin{aligned} pv &= RT \\ h &= u + pv \end{aligned}\right\} \Longrightarrow \quad c_p = c_v + R$$

$$c_v = \frac{\partial u}{\partial T}$$

c_v constant

$$\Longrightarrow \quad u = c_v(T - T_0)$$

reference temperature

$$h = u + RT \quad \Longrightarrow$$

h is also function of T alone

$$c_p = \frac{\partial h}{\partial T}$$

$$\Longrightarrow \quad h = c_p(T - T_0) + RT_0$$

c_p constant due to $c_p = c_v + R$

$$du = T\,ds - p\,dv \quad \Longrightarrow \quad ds = \frac{du}{T} + p\frac{dv}{T} = c_v\frac{dT}{T} + R\frac{dv}{v}$$

$$\Longrightarrow \quad s = c_v \log\frac{T}{T_0} + R\log\frac{v}{v_0} \quad \Longrightarrow \quad T = T_0 e^{\frac{s}{c_v}} \left(\frac{v}{v_0}\right)^{-\frac{R}{c_v}}$$

integration of the 1-form

$$\mathrm{d}h = T\ \mathrm{d}s + v\ \mathrm{d}p \quad \Longrightarrow \quad \mathrm{d}s = \frac{\mathrm{d}h}{T} - v\frac{\mathrm{d}p}{T} = c_p\frac{\mathrm{d}T}{T} - v\frac{\mathrm{d}p}{T}$$

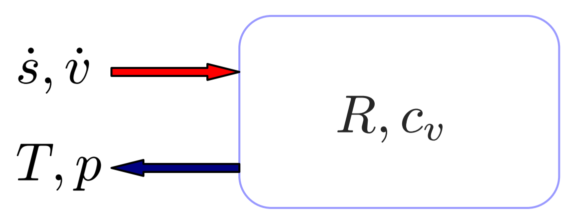
$$= c_p\frac{1}{RT}(p\ \mathrm{d}v + v\ \mathrm{d}p) - \frac{v}{T}\mathrm{d}p = c_p\frac{\mathrm{d}v}{v} + \frac{v}{T}\left(\frac{c_p}{R} - 1\right)\mathrm{d}p = c_p\frac{\mathrm{d}v}{v} + c_v\frac{\mathrm{d}p}{p}$$

integration of the 1-form

$$\Longrightarrow \quad s = c_p \log\frac{v}{v_0} + c_v \log\frac{p}{p_0} \quad \Longrightarrow \quad p = p_0 e^{\frac{s}{c_v}}\left(\frac{v}{v_0}\right)^{-\frac{c_p}{c_v}}$$

$$\left.\begin{aligned} p &= p_0 e^{\frac{s}{c_v}}\left(\frac{v}{v_0}\right)^{-\frac{c_p}{c_v}} \\[2ex] T &= T_0 e^{\frac{s}{c_v}}\left(\frac{v}{v_0}\right)^{-\frac{R}{c_v}} \end{aligned}\right\}$$

constitutive equations for
a perfect gas in all-integral form



Exercise: compute the constitutive equations
for the other three causality patterns.

Chemical engineering:

transport phenomena

quantities of substances vary with time

Requires an extension of the basic
thermodynamic bond graph framework

Geometric Network Modeling and Control of Complex Physical Systems

IST-2001-34166

stirred reaction tanks

fuel cells

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