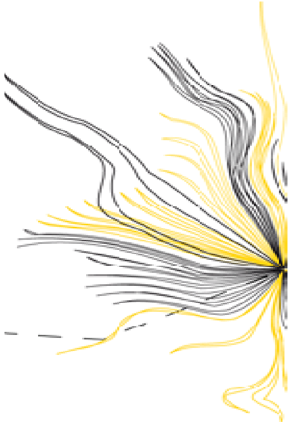
UNIVERSITY OF TWENTE.

ON THE IMPORTANCE OF A PROPER USE OF ENERGY FUNCTIONS IN TRANSPORT MODELS

Peter Breedveld
University of twente
Enschede
Netherlands
p.c.breedveld@utwente.nl



SETTING THE STAGE… VIEWPOINT

- **Context of justification (‘world of proofs’): *model manipulation* (mathematics, mathematical physics)**

versus

- **Context of discovery/explanation: *modeling* as a decision process, abstraction (engineering physics)**

SETTING THE STAGE… VIEWPOINT

- **Herein focus on *reduction* by**
  - **making well-based *initial modeling decisions***
  - ***structured* approach**
  - **variable *categorization* based on physical properties**
  - **tools/*notation* that support modeling decisions**
  - ***INSIGHT* in physical behavior**
- **Mathematical *result* still open for further reduction!**

SETTING THE STAGE… TERMINOLOGY

- **Ideal concepts (‘storage’, ‘transformation’, etc.): mental pictures**
- **Communication: depicting imaginary concepts into visible images – ideal ‘elements’**
- **Potential confusion of**
  - **ideal elements with tangible components**
  - **topological structure with spatial (geometrical) structure**

    (see Walter Lewin’s lecture about Faraday versus Kirchhoff:
    part 1: http://www.youtube.com/watch?v=eqjl-qRy71w&NR=1,
    part 2: http://www.youtube.com/watch?v=1bUWcy8HwpM&feature=related)

EXAMPLE: FARADAY'S LAW

$$\oint_C E \cdot dl = -\frac{d}{dt}\iint_S B \cdot dA$$

$$\oint_C E \cdot dl + \frac{d}{dt}\iint_S B \cdot dA = 0$$

- **Physicists: d*B*/d*t* = 0 for Kirchhoff's voltage law to hold (*geometrical* interpretation)**
- **Electrical engineers, graph theoreticians: dλ/d*t* is a voltage (*topological* interpretation of the quasistationary situation)**

$$\frac{d\lambda}{dt} = n\frac{d\Phi}{dt} = n\frac{d}{dt}\iint_S BdA$$

- **i.o.w.: topological structure is NOT EQUAL TO geometrical structure (Lewin's confusion)**

‘LUMPED’ VERSUS ‘DISTRIBUTED’

- **Ideal elements are *conceptual* ‘lumps’**
- **Distributed system models treat *configuration* space in a continuous way**
  but
  still use *conceptually* ‘lumped’ concepts(!):
  - **various balance equations (momentum, mass, etc.)**
  - **dissipation relations**
  - **etc.**
- **All conceptually separated…**

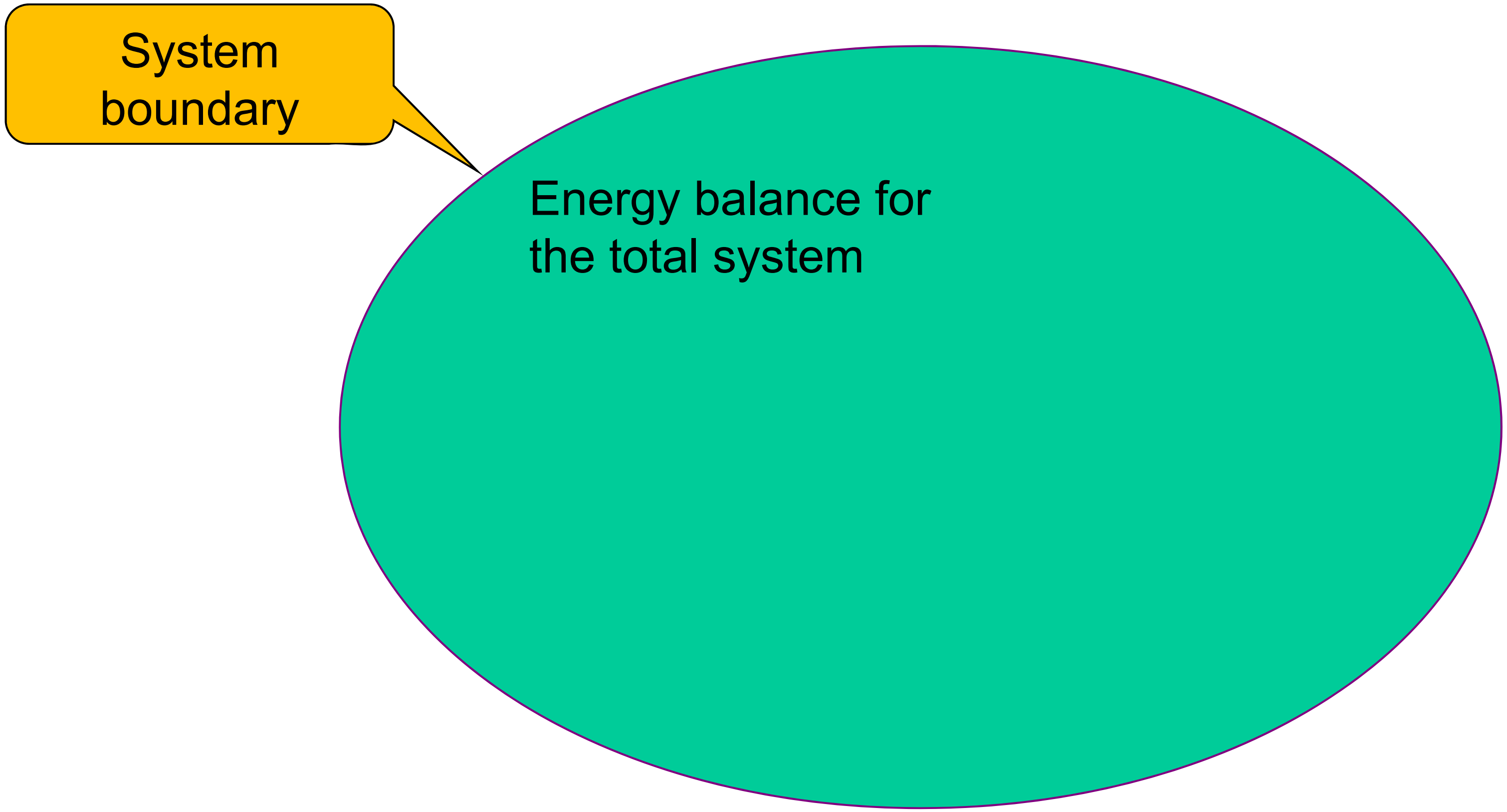
PREREQUISITES

- **Basic physical concepts: e.g. quantities for which a conservation principle holds (momentum, charge, etc.)**
- **Physical interaction implies energy exchange = = power ('through' *conceptual* ports)**
  - **even information exchange requires low power: back effect is (made) negligible (e.g. sensor & amplifier)**
- **Eulerian vs. Lagrangian coordinates ('view point')**
- **Legendre transforms**
- **Basics of (ir-)reversible thermodynamics**

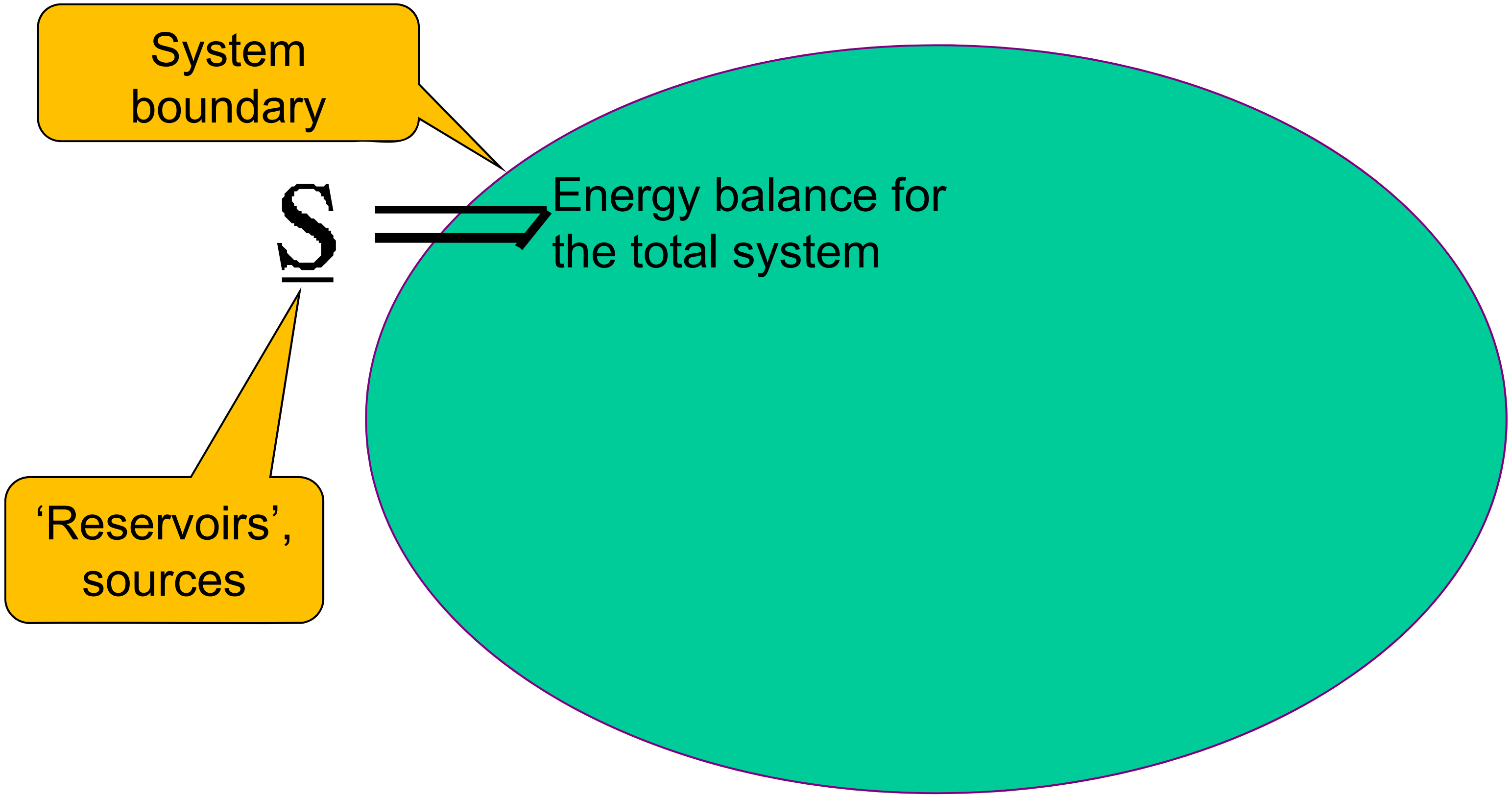
‘PITCH’ OF POINTS TO MAKE

- **separation between *configuration* and *energy* states: more insight**
- **system boundary definitions may be *mixed*: Eulerian vs Lagrangian**
- **concept of energy *density* (material of spatial) synonymous with first degree homogeneous energy function of all possible extensive states *in principle***
- **energy-based modeling approach/notation:**
  - **automatically satisfies fundamental principles of physics when all grammar rules are obeyed**
  - **systematic approach to the dynamic behavior of all properties that may be *convected* in principle (e.g. momentum, electric charge, etc.);**
- **generalized thermodynamic framework of variables more general than Hamiltonian (generalized mechanical) framework:**
  - **some domains have no dual storage**

THERMODYNAMIC APPROACH



THERMODYNAMIC APPROACH



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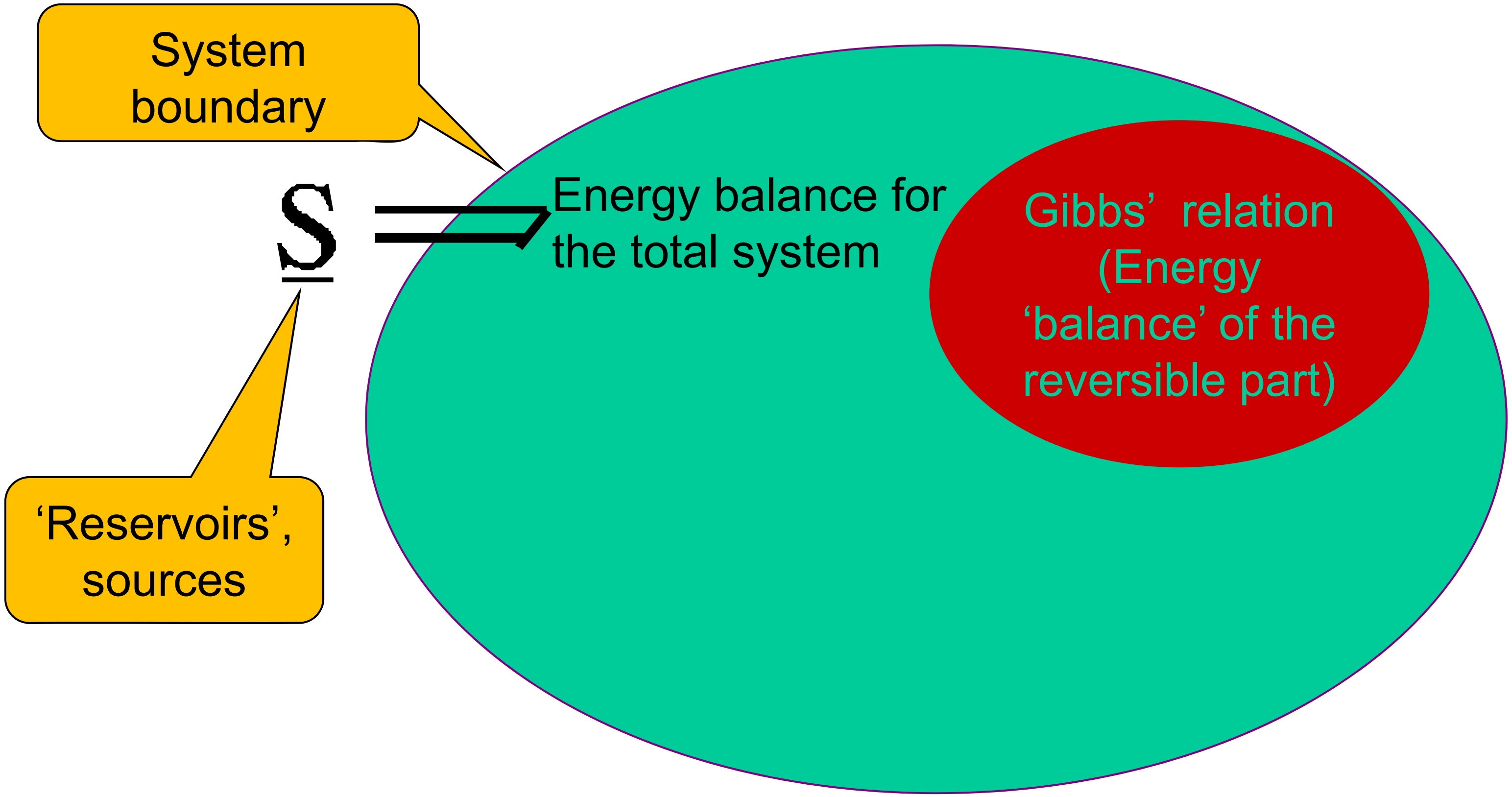

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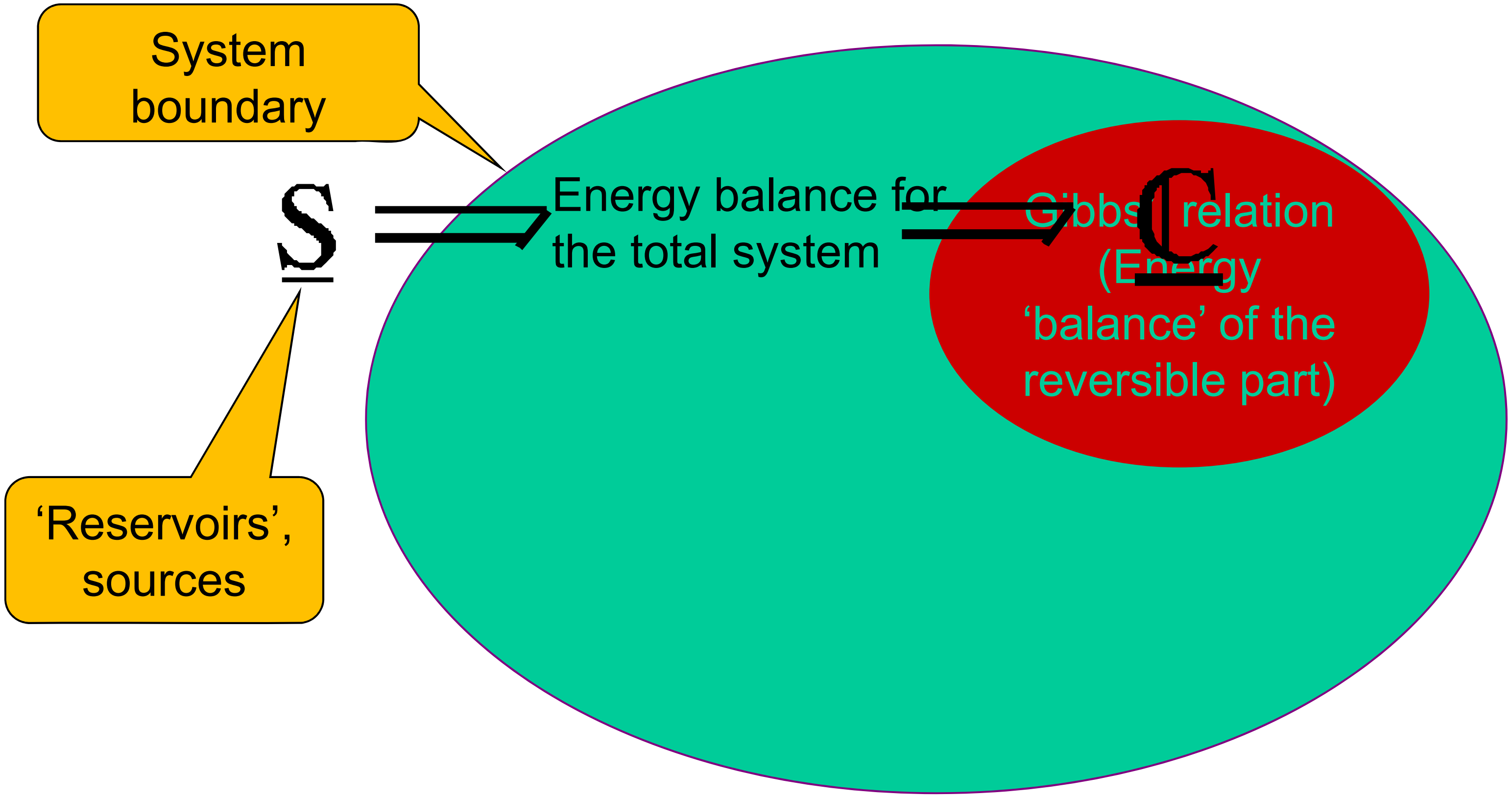

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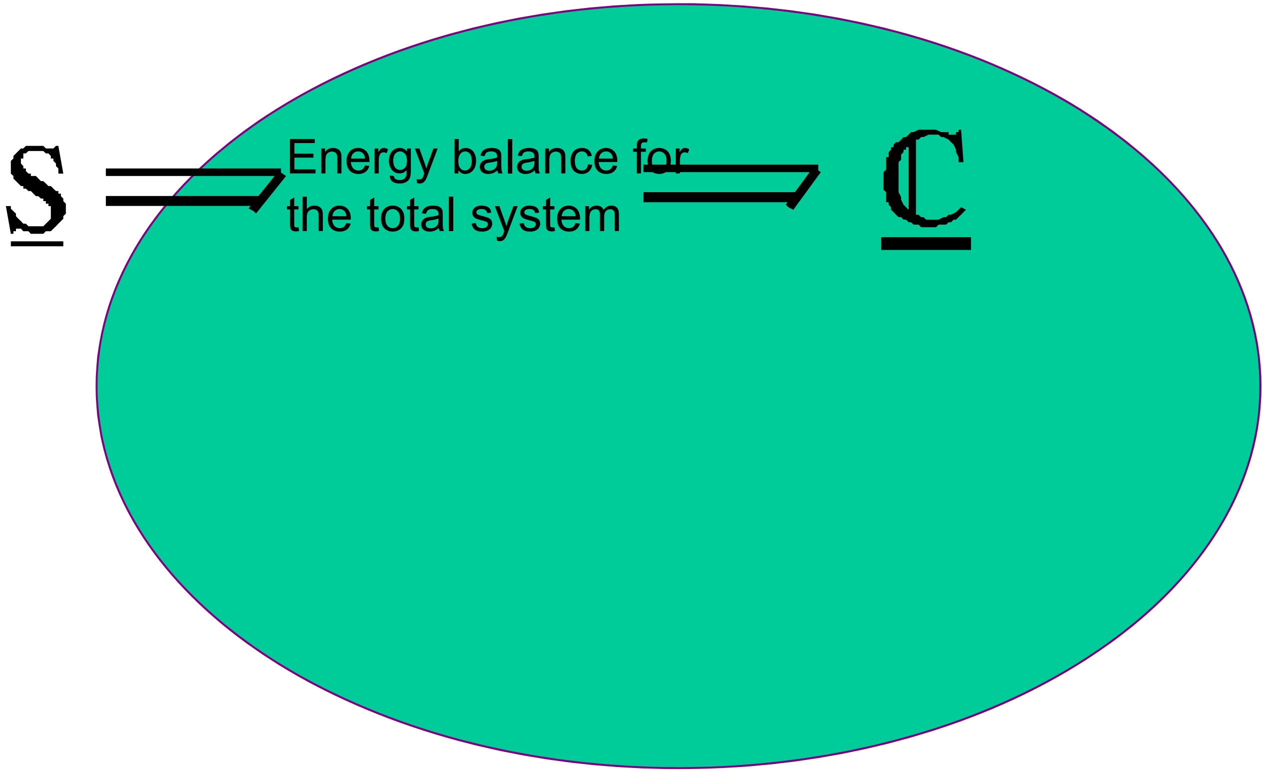

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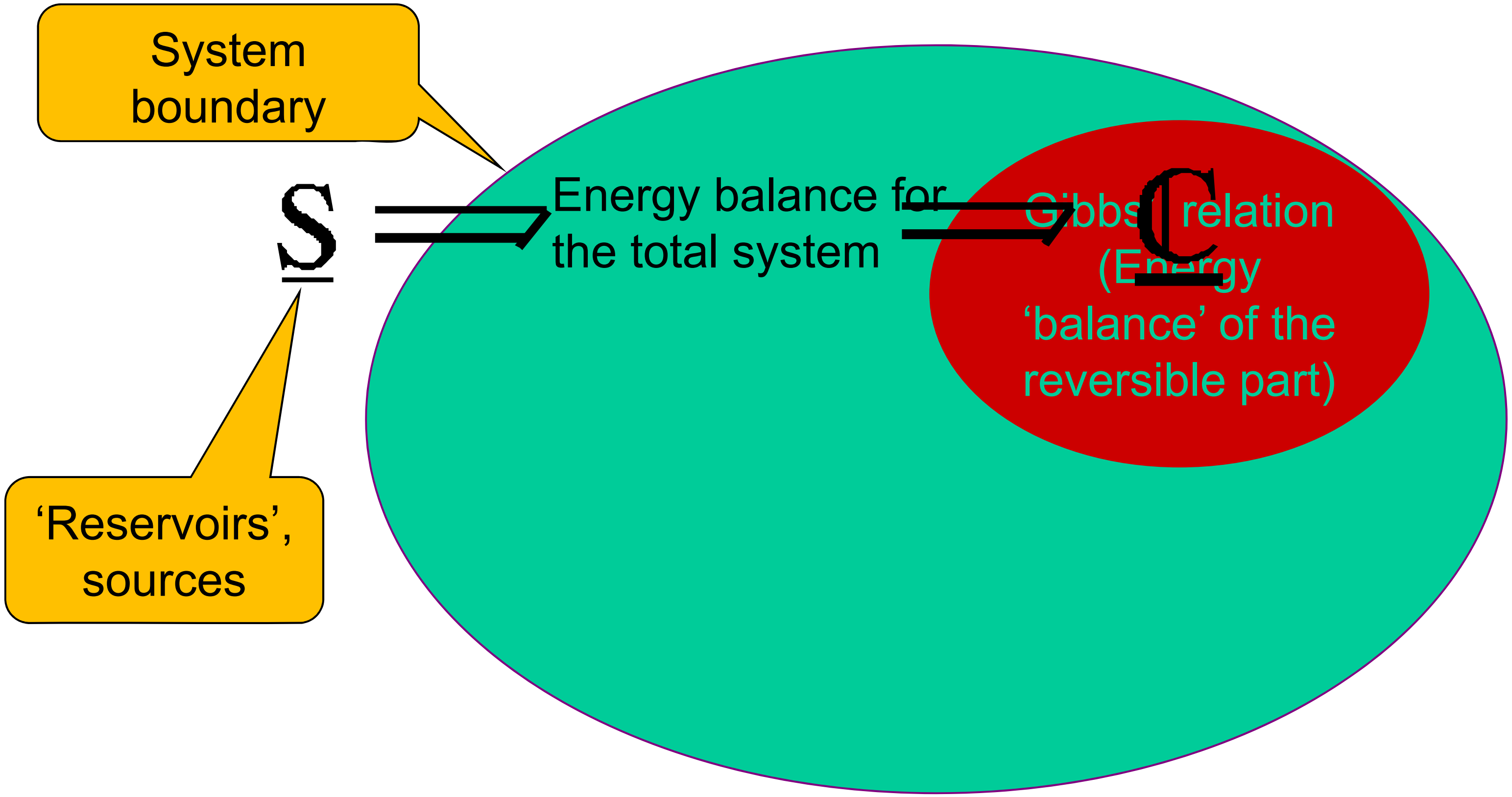

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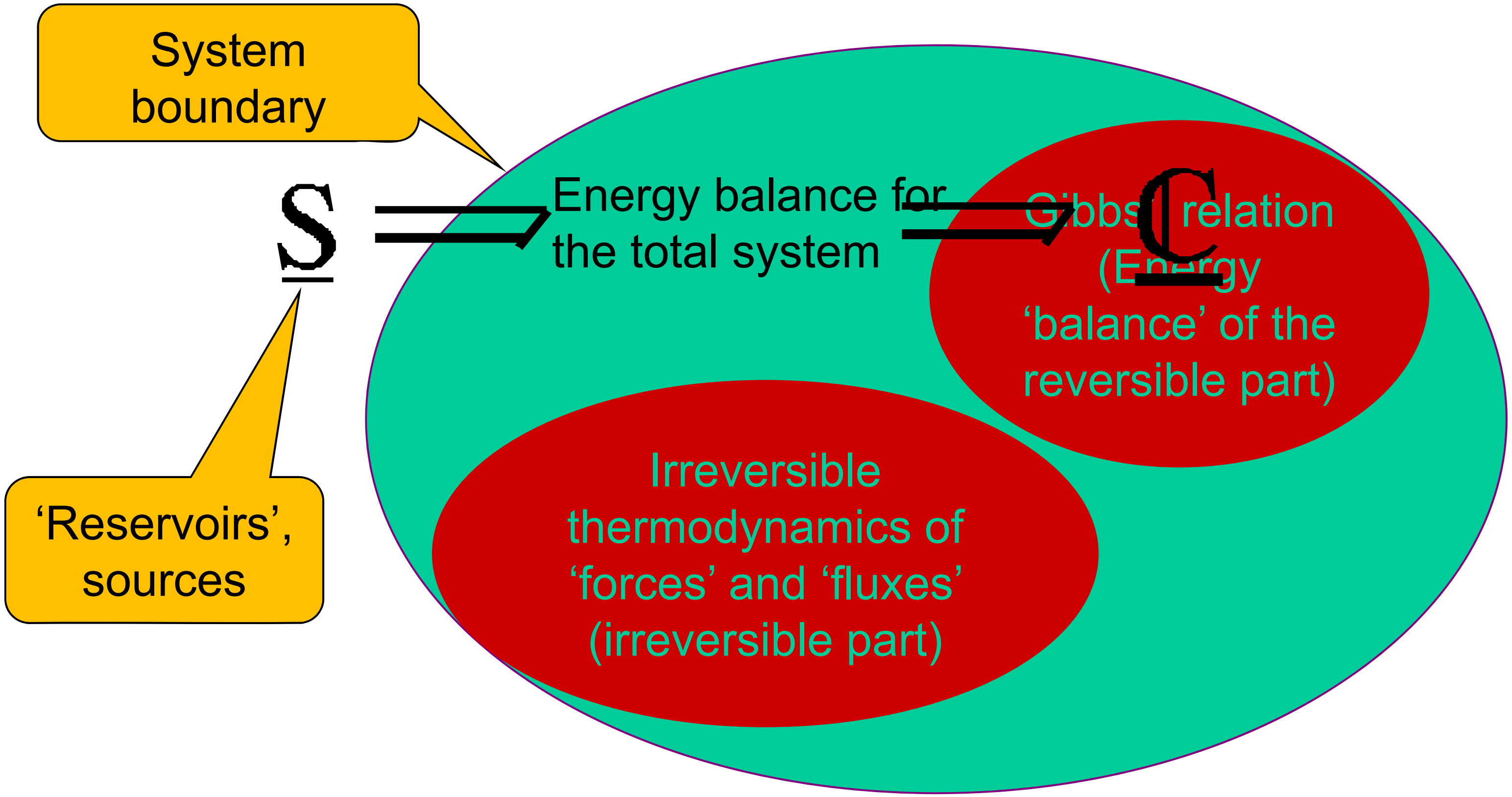

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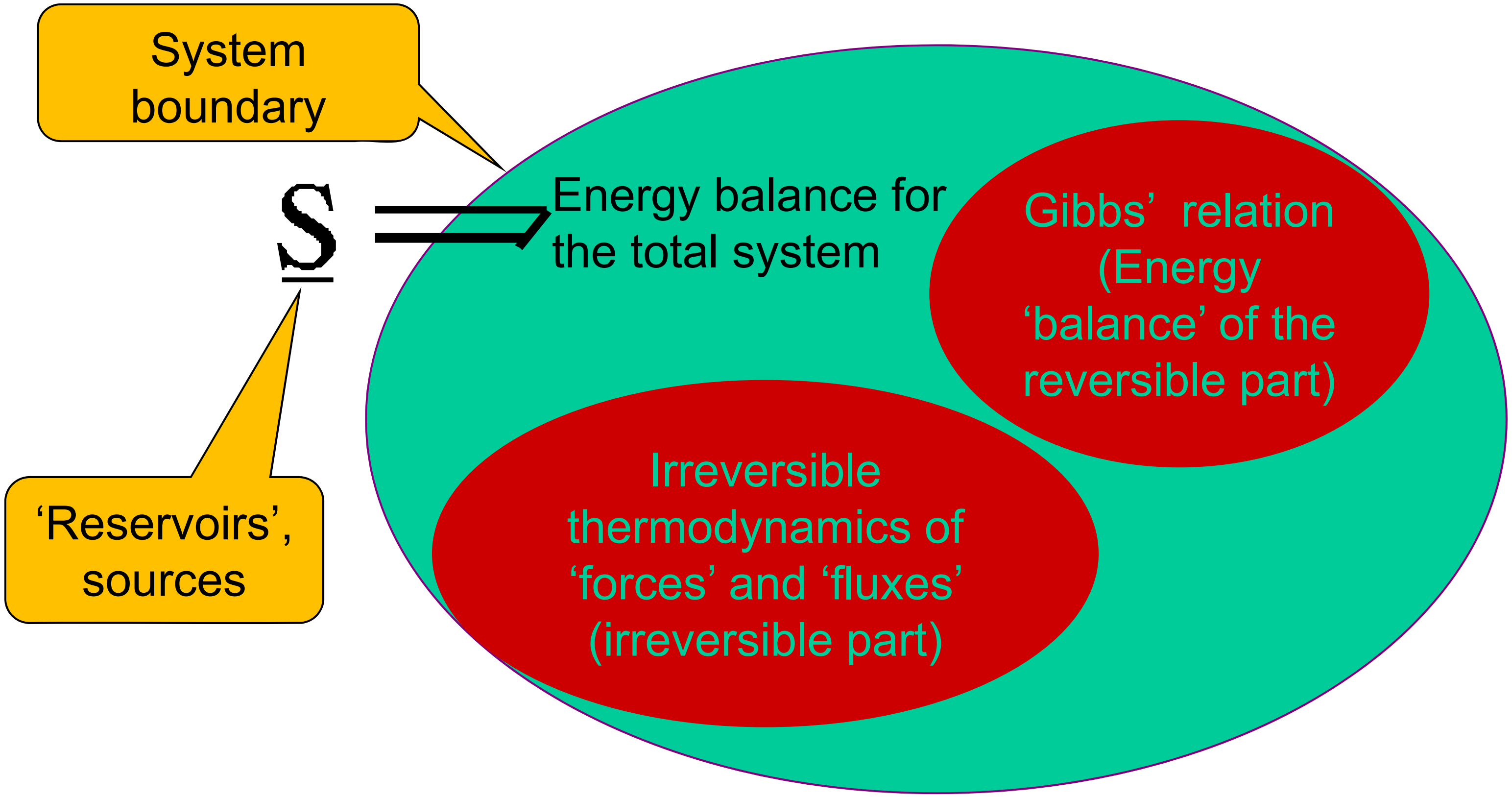

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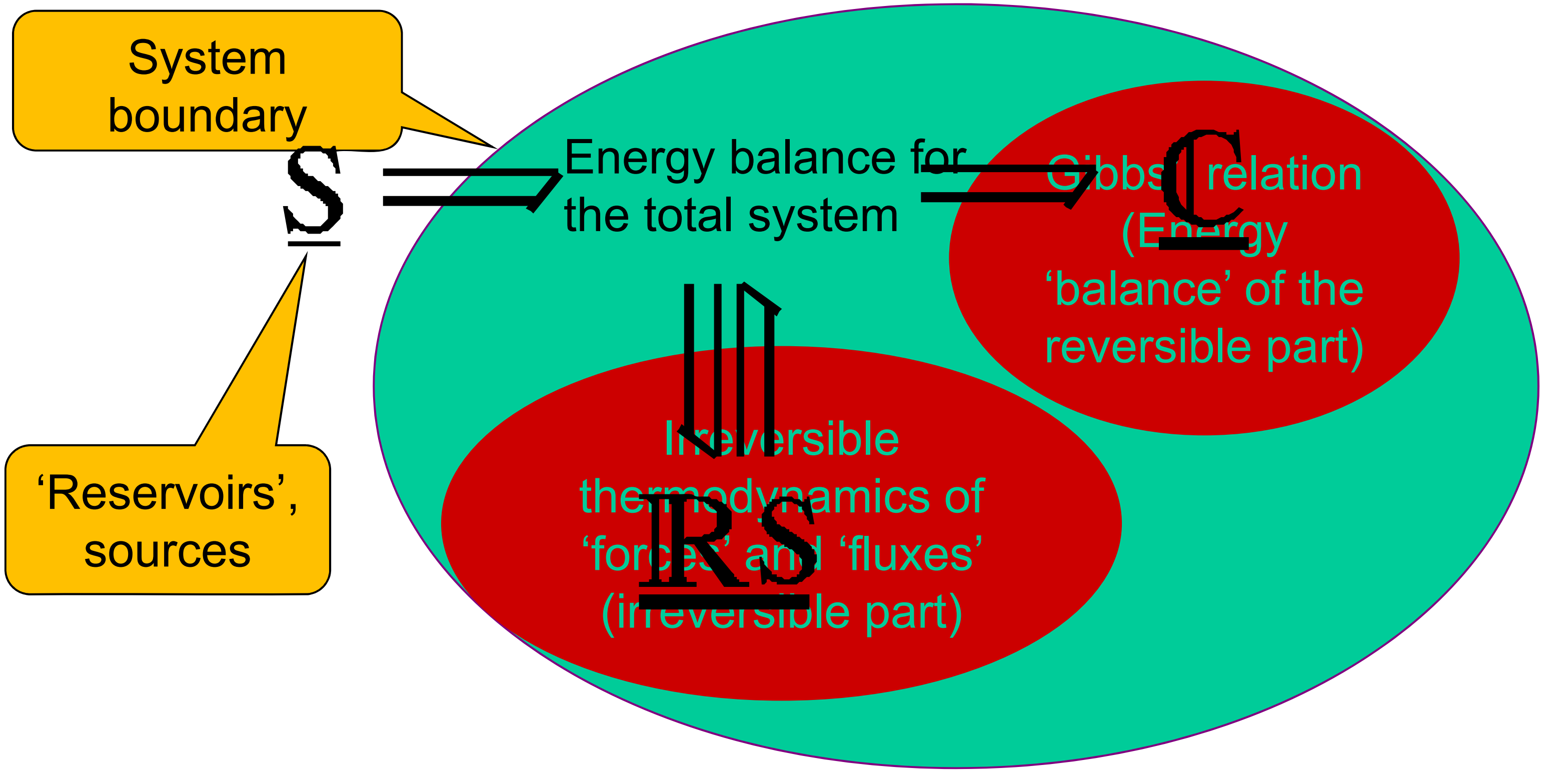

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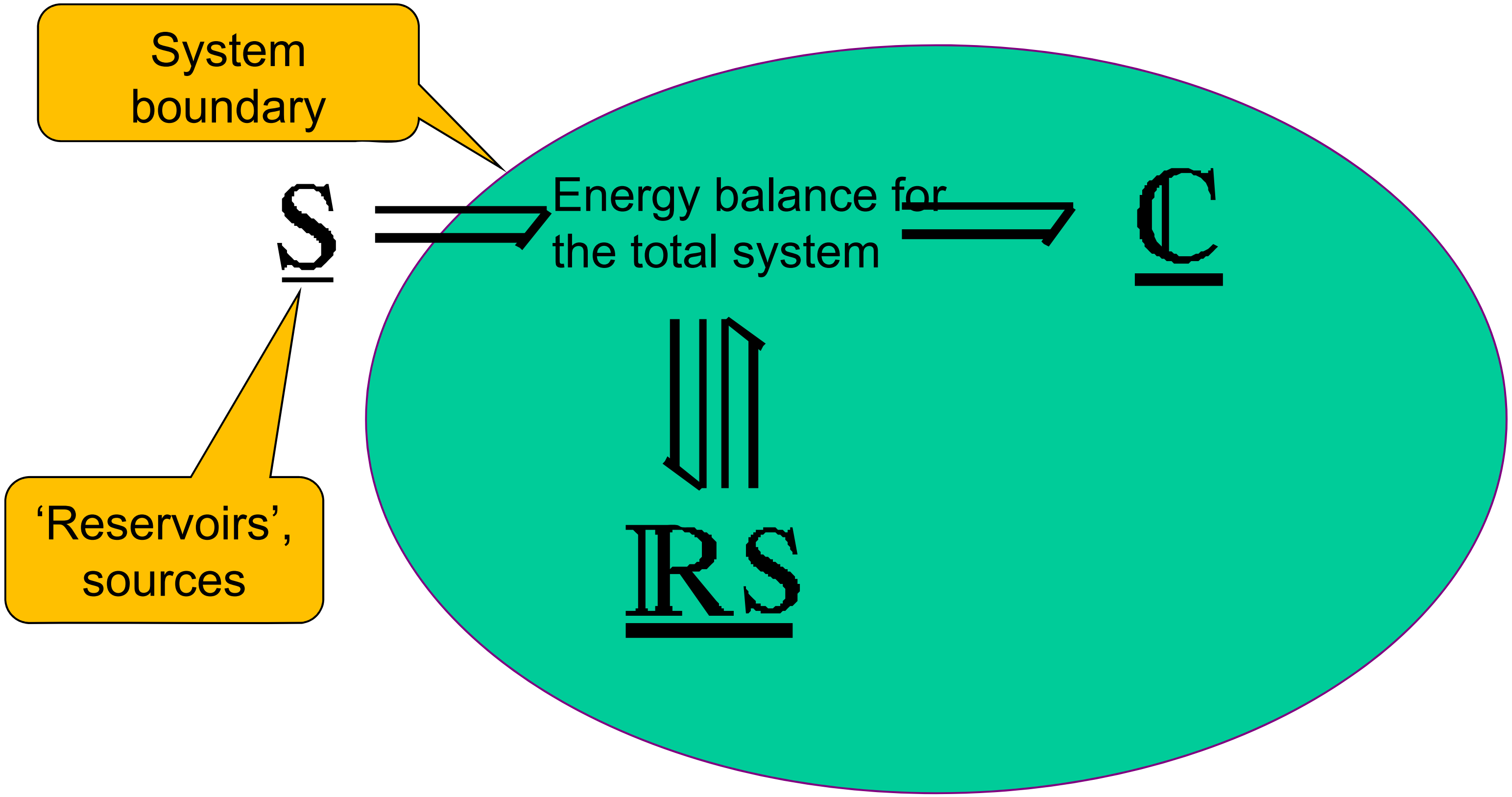

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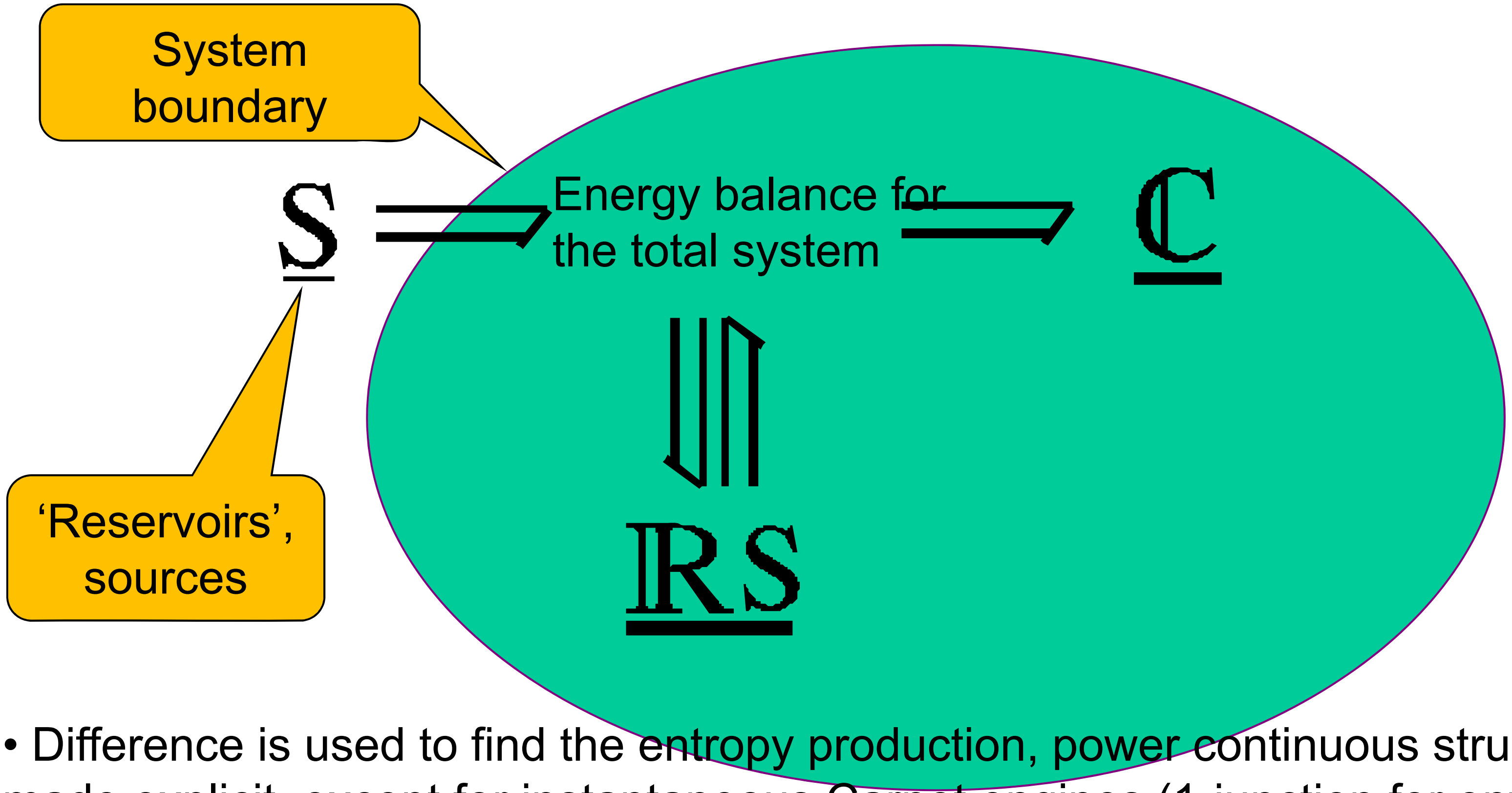
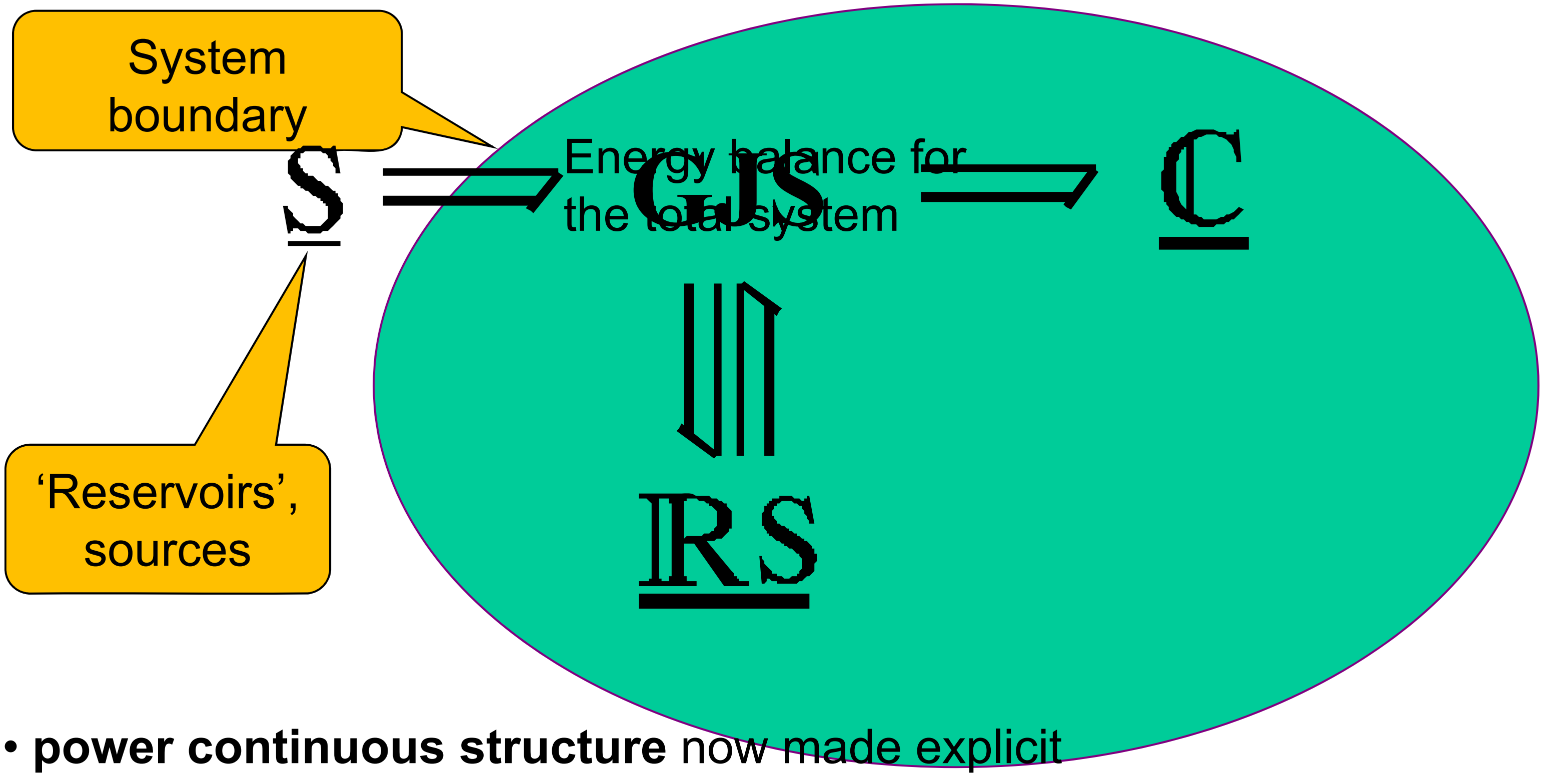


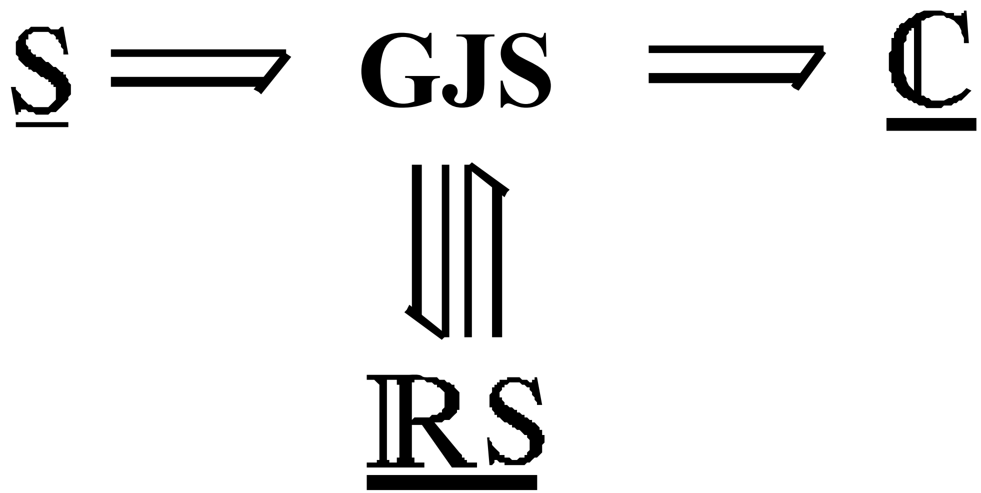
• Difference is used to find the entropy production, power continuous structure not made explicit, except for instantaneous Carnot engines (1-junction for entropy flow)

NETWORK THERMODYNAMIC APPROACH



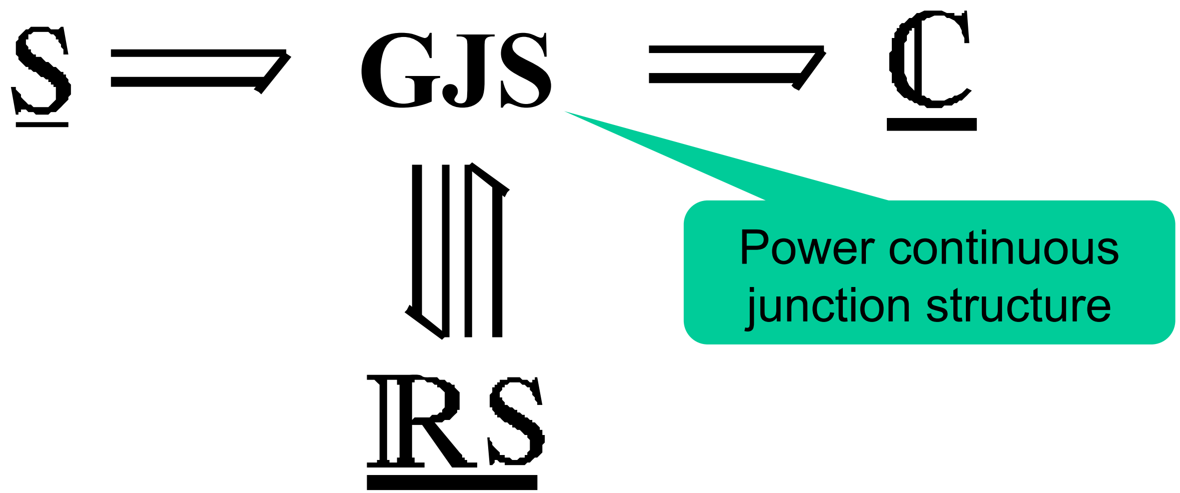
• **power continuous structure** now made explicit

NETWORK THERMODYNAMIC APPROACH



• simplified picture, containing the same information…

NETWORK THERMODYNAMIC APPROACH



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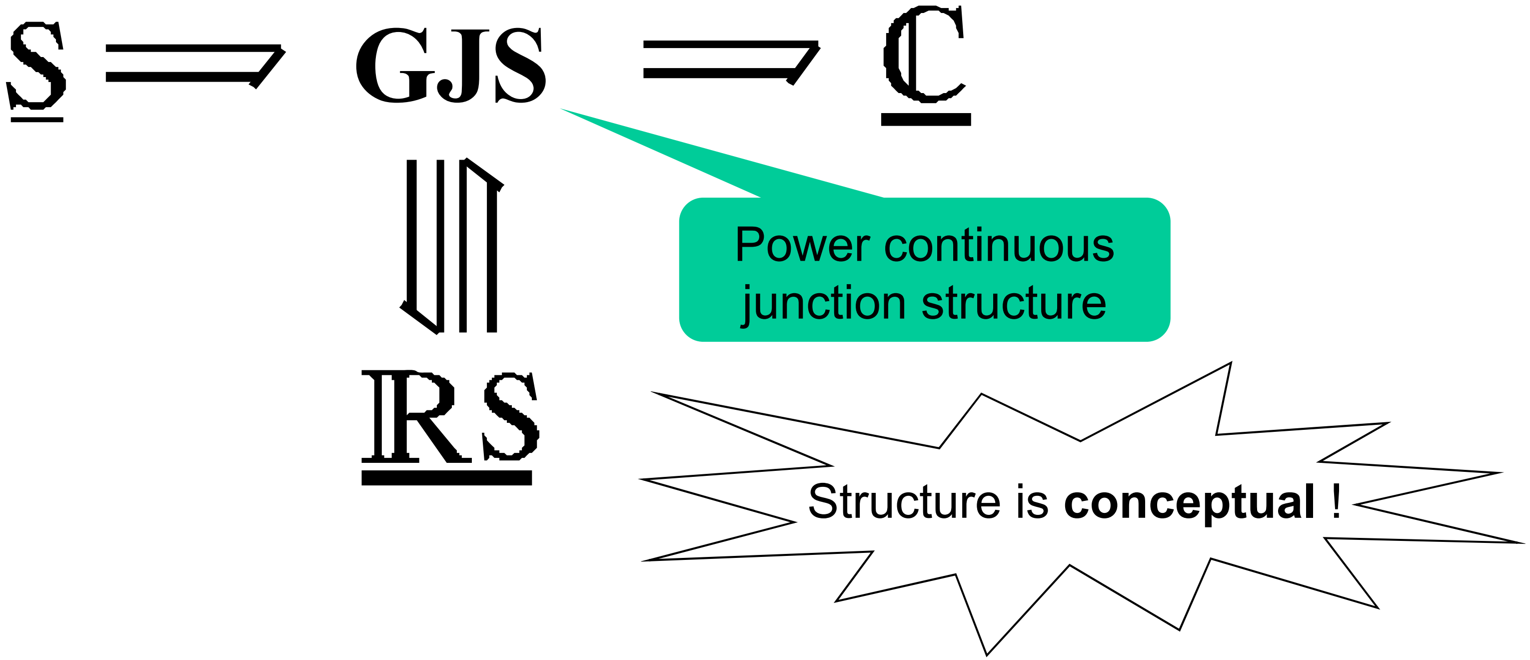
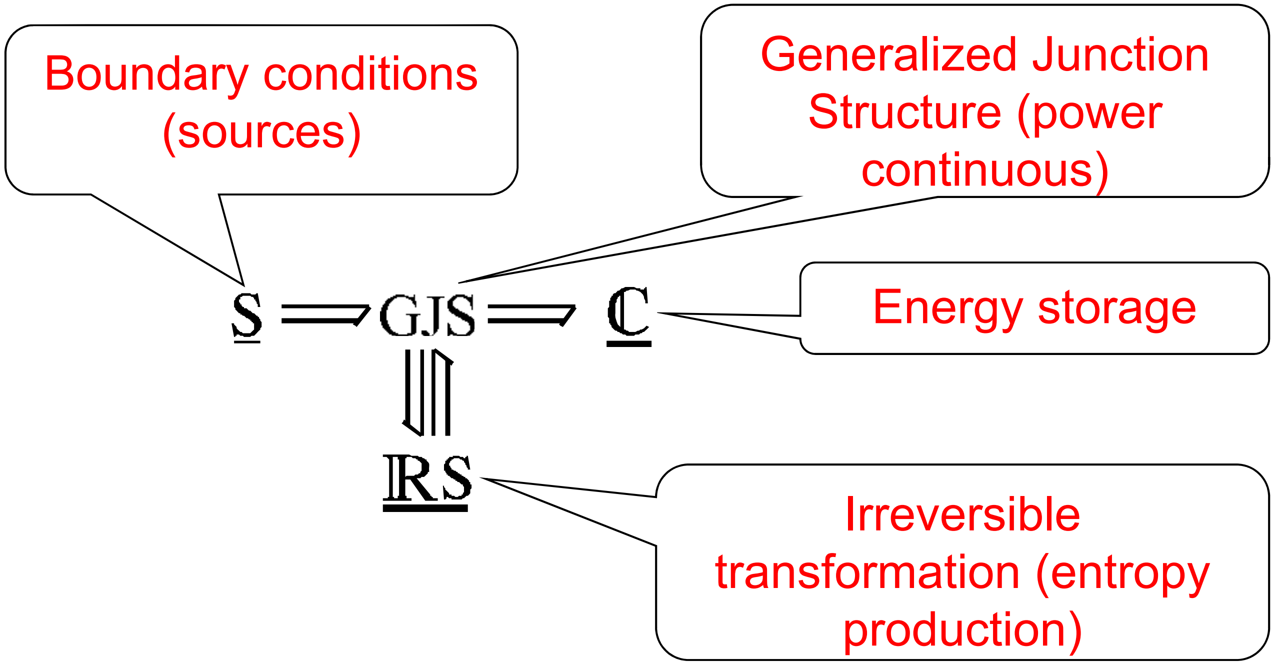


BASIC MODEL STRUCTURE (GENERALIZED BOND GRAPH)



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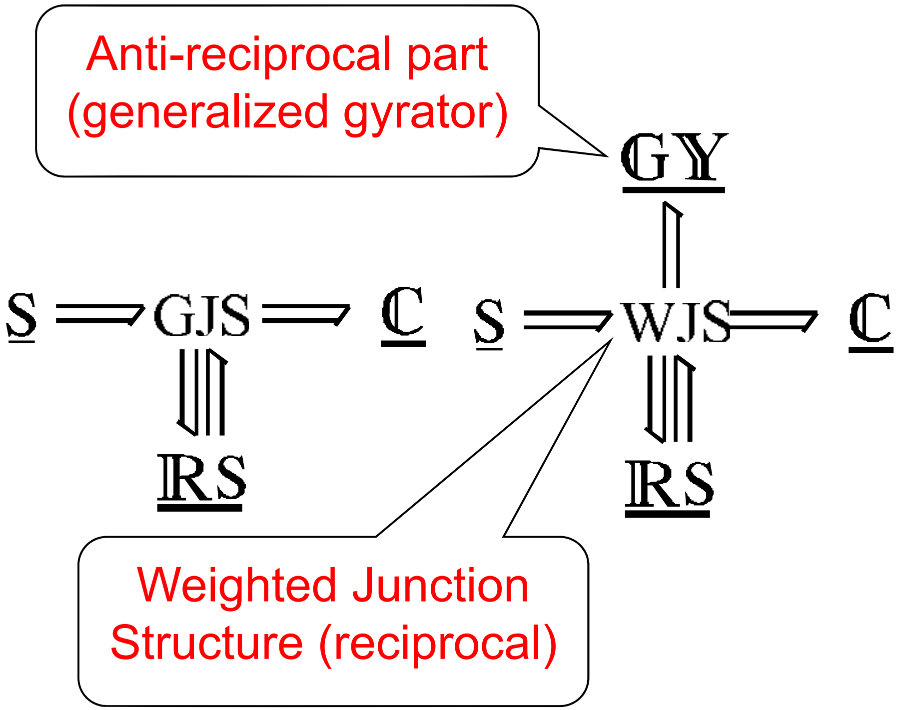

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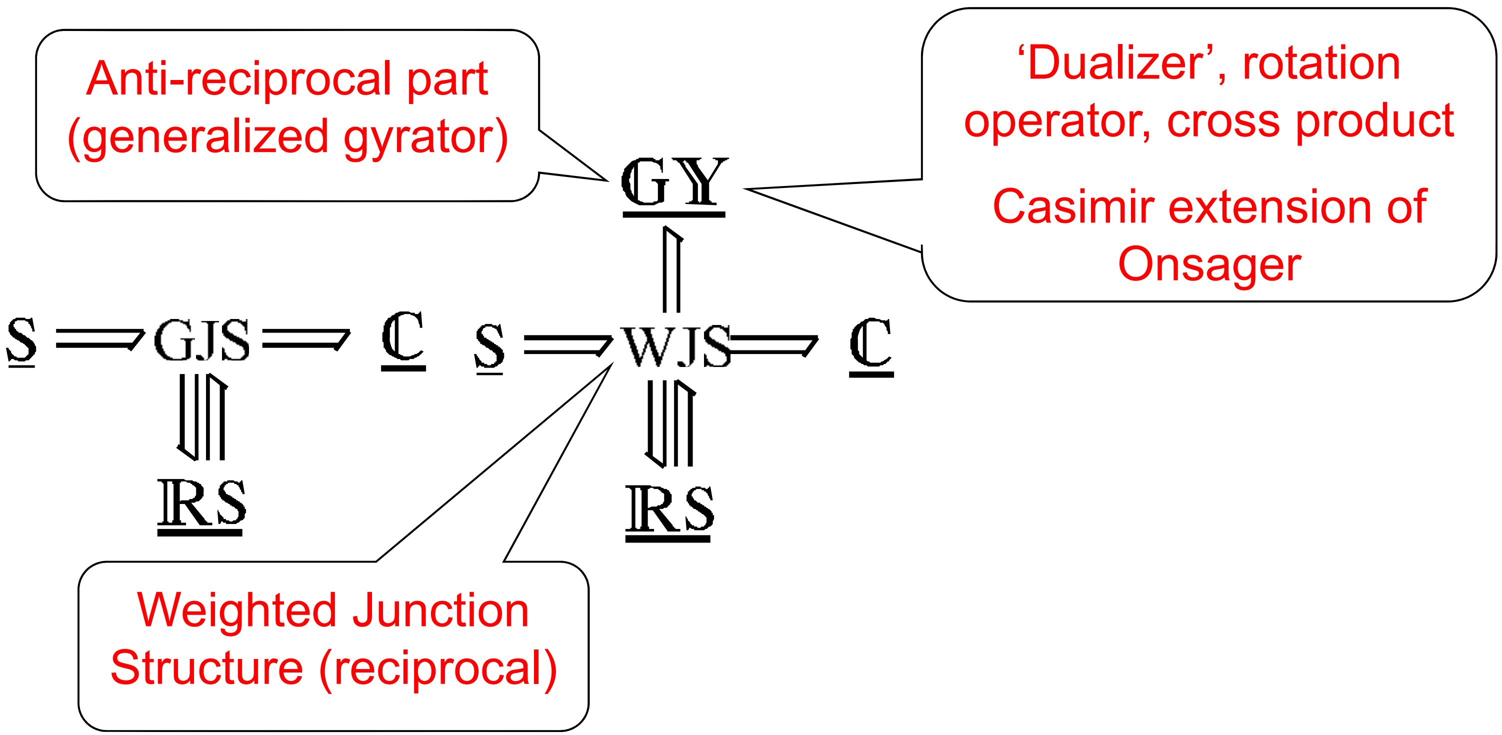

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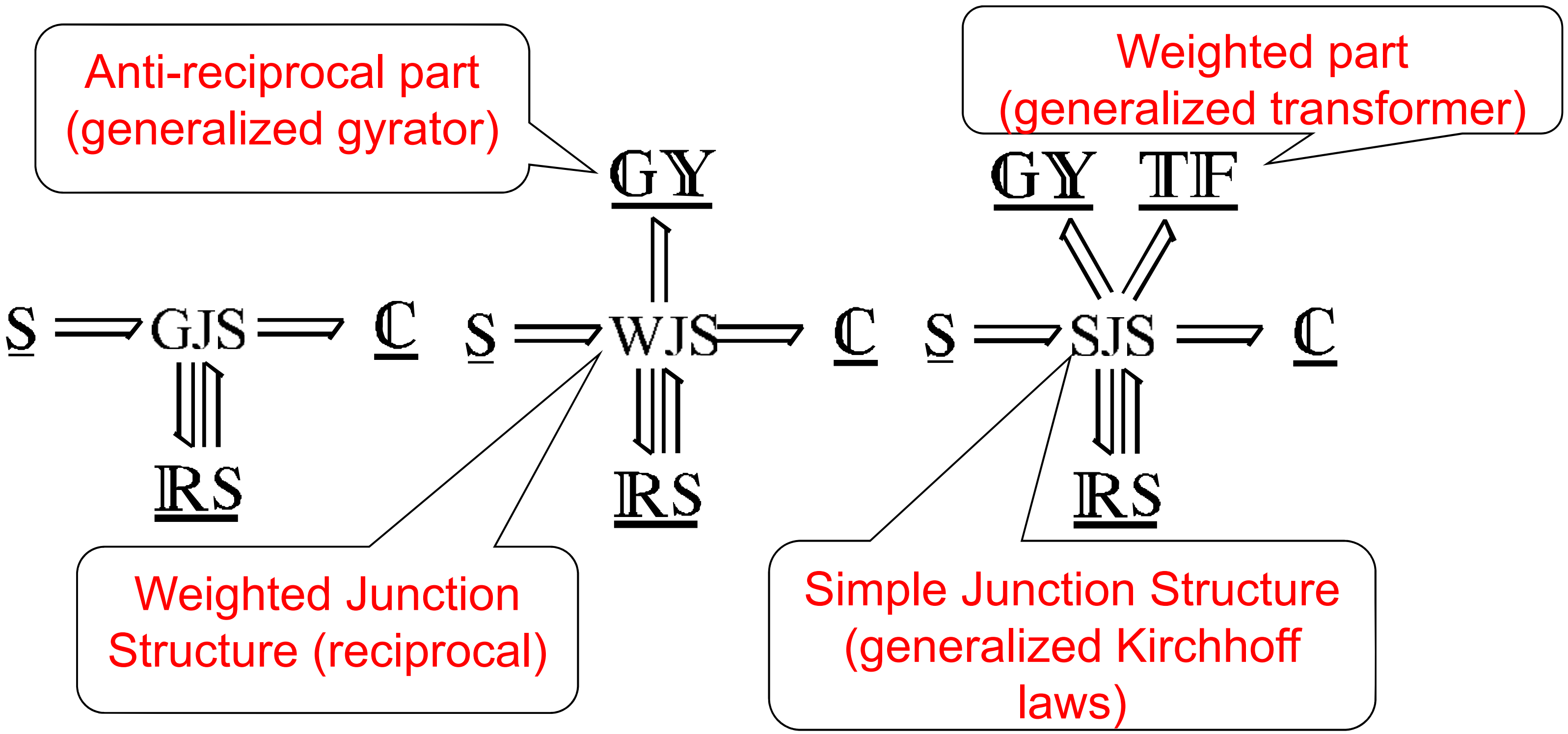


CONFIGURATION INFLUENCE ON ENERGETIC STRUCTURE

- can 'become' an **additional energy state**: geometric parameter in storage relation results in a force

$$F\left(q,x\right)=\frac{\partial E\left(q,x\right)}{\partial x}$$

  - examples: LVDT, electret microphone, relay, (ideal) gas etc. (MP C)
  - *cycles allow transduction*
  - changes of causality correspond to Legendre transforms!! (relation to dissipation)
- can **modulate** an energy relation
  - examples: crank-slider *mechanism*, etc. (MTF)
- can **switch** a contact (or behavior)

ENERGY AS STARTING POINT

- **Energy**
  - $E = E\left(\underline{q}\right) = E\left(q_1,\ldots,q_i,\ldots q_n\right)$
  - Homogeneous function of set of extensive state variables
- In ('generalized') *mechanics* : Hamiltonian
  - $E = H\left(\underline{q},\underline{p}\right) = H\left(q_1,\ldots,q_i,\ldots q_k,p_1,\ldots,p_i,\ldots p_k\right)$
- In *thermodynamics* of 'simple' systems: internal energy
  - $E = U\left(\underline{q}\right) = U\left(V,S,N\right)$
  - more species: $E = U\left(\underline{q}\right) = U\left(V,S,\underline{N}\right) =$

$$= U\left(V,S,N_1,\ldots,N_i,\ldots,N_m\right) =$$
$$= U\left(V,S,N_1,\ldots,N_i,\ldots,N_{m-1},N\right)$$

ENERGY-BASED MODEL FORMULATION

- **Energy and power: domain independent concepts**
- **An energy function of a set of *k* conserved states *q*:** $E\left(q_1,\ldots q_i,\ldots q_k\right)$
- **Result in a power:**

$$P=\frac{dE\left(q_1,\ldots q_i,\ldots q_k\right)}{dt}=\sum_{i=1}^{k}\frac{\partial E\left(q_1,\ldots q_i,\ldots q_k\right)}{\partial q_i}\frac{dq_i}{dt}=\sum_{i=1}^{k}e_i f_i$$

- **where** $f_i=\frac{dq_i}{dt}$ **is an equilibrium-establishing variable or *flow***
- **and** $e_i\left(q_1,\ldots q_i,\ldots q_k\right)=\frac{\partial E\left(q_1,\ldots q_i,\ldots q_k\right)}{\partial q_i}$ **is an equilibrium-determining variable or *effort***

- ***This distinction is lost in a Hamiltonian framework!***

ENERGY-BASED MODELING APPROACH

- **Note that a balance equation for a conserved, extensive state**

$$\frac{dq}{dt} = \sum \varepsilon f$$

with $\varepsilon = \pm 1$ depending on direction w.r.t. positive orientation

- **May now be written as**

$$\sum \varepsilon f = 0$$

GENERALIZED THERMODYNAMIC FRAMEWORK OF VARIABLES

	f *flow*	e *effort*	$q = \int f \, \mathrm{d}t$ *generalized state*
electric	i current	u voltage	$q = \int i \mathrm{d}t$ charge
magnetic	u voltage	i current	$\lambda = \int u \mathrm{d}t$ magnetic flux linkage
thermal	T temperat ure	f_S entropy flow	$S = \int f_S \mathrm{d}t$ entropy
chemical	μ chemical potential	f_N molar flow	$N = \int f_N \mathrm{d}t$ number of moles

GENERALIZED THERMODYNAMIC FRAMEWORK OF VARIABLES

	f *flow*	e *effort*	$q = \int f \, dt$ *generalized state*
elastic/potential translation	v velocity	F force	$x = \int v dt$ displacement
kinetic translation	F force	v velocity	$p = \int F dt$ momentum
elastic/potential rotation	ω angular velocity	T torque	$\theta = \int \omega dt$ angular displacement
kinetic rotation	T torque	ω angular velocity	$b = \int T dt$ angular momentum
elastic hydraulic	φ volume flow	p pressure	$V = \int \varphi dt$ volume
kinetic hydraulic	p pressure	φ volume flow	$\Gamma = \int p dt$ momentum of a flow tube

MECHANICAL FRAMEWORK OF VARIABLES

	f *flow*	e *effort*	$q = \int f \, dt$ *generalized displacement*	$p = \int e \, dt$ *generalized momentum*
electromagnetic	i current	u voltage	$q = \int i dt$ charge	$\lambda = \int u dt$ magnetic flux linkage
mechanical translation	v velocity	F force	$x = \int v dt$ displacement	$p = \int F dt$ momentum
mechanical rotation	ω angular velocity	T torque	$\theta = \int \omega dt$ angular displacement	$b = \int T dt$ angular momentum
hydraulic	φ volume flow	p pressure	$V = \int \varphi dt$ volume	$\Gamma = \int p dt$ momentum of a flow tube

SYNTHESIS OF MECHANICAL & THERMODYNAMIC FRAMEWORK

Mechanics:	Thermodynamics:
Two types of storage	One type of storage
Oscillatory behavior (damped): C-I(-R)	Only relaxation behavior: C-R
Split domains (therm.) and couple by SGY (mech.): C-SGY-C	

GENERALIZED THERMODYNAMIC FRAMEWORK

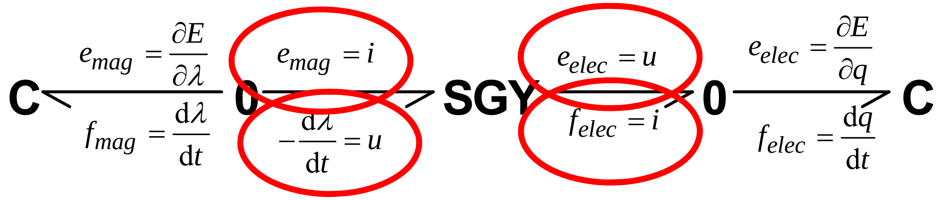
UNRESOLVED ISSUE?

- What is analog to what?
  - Mass and coil or mass and capacitor?
    or
  - Spring and capacitor or spring and coil?
- Long debates since mid thirties…

PHYSICAL MEANING OF THE SYMPLECTIC GYRATOR

- Electrical network (q,λ):
  - ***Only*** if **quasi-stationary** (non-radiating), Maxwell's equations reduce to:

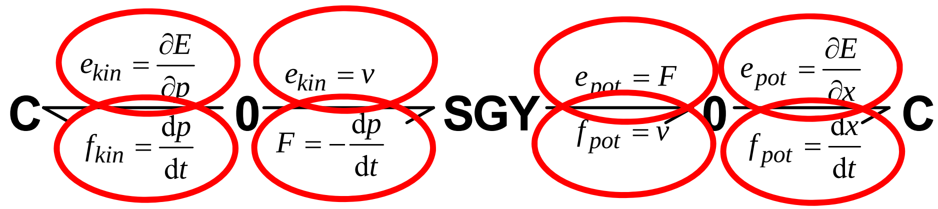
$$-\frac{\mathrm{d}\lambda}{\mathrm{d}t} = u \qquad e_{mag} = i$$



  - Dualizing effect!

PHYSICAL MEANING OF THE SYMPLECTIC GYRATOR

- Mechanical (x,p)
  - *Only* when in **inertial** frames, i.e. when Newton's 2nd law holds:



$$F = -\frac{dp}{dt}$$

'SPECIAL' STATES

Position/displacement

- has a *dual* nature:
  - energy state (related to a conservation or symmetry principle like all other states)
  - configuration state

Matter

- convects all matter-bound properties (not 'available volume'!)
- conjugate intensity depends on other intensities (Gibbs-Duhem)
- *boundary criterion*

Volume

- *boundary criterion*

Entropy

- can be 'locally' *produced* & is only 'locally' conserved (conceptual separation!)

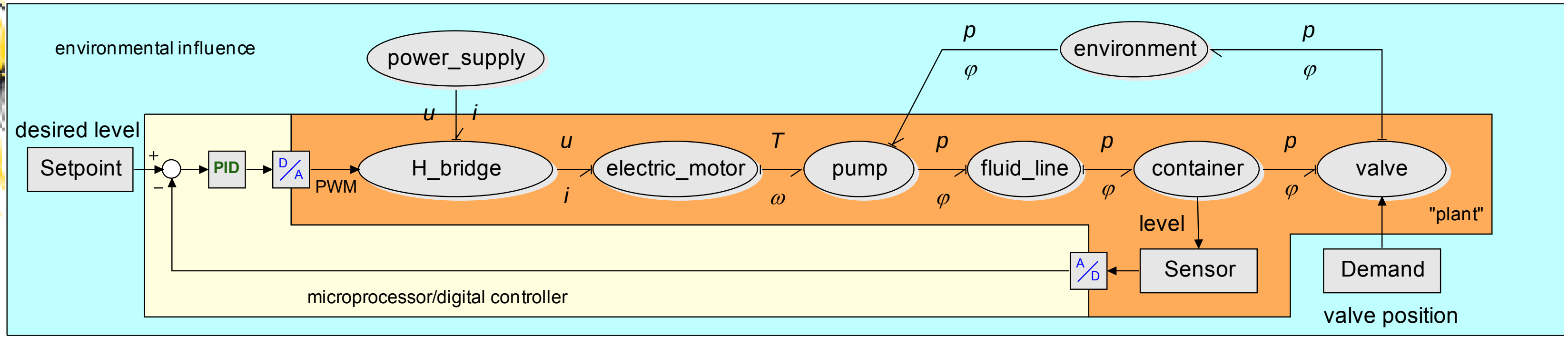
SYSTEM (BOUNDARY) DEFINITION

- Open (thermodynamic) systems
- **d*N* = 0** (d*m*=*MdN*=*0*) : ‘Lagrangian coordinates’, material boundary criterion:

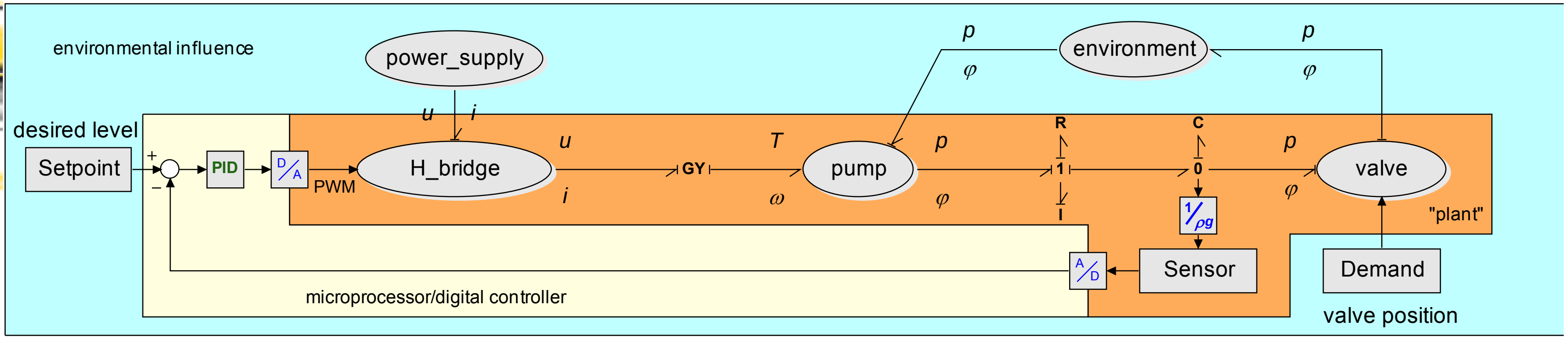
  N not a state
- **d*V* = 0** (*Adx*=*0*): ‘Eulerian coordinates’ (control volume, spatial boundary criterion):

  V not a state
- Almost always **mixed** boundaries:
  N and ***V*** **remain states** for system under study!
- **Tangible system:** *globally Lagrangian, locally Eulerian*
- **Network of subsystems**: *globally Eulerian*, *locally Lagrangian* (e.g. network of elastic tubes)

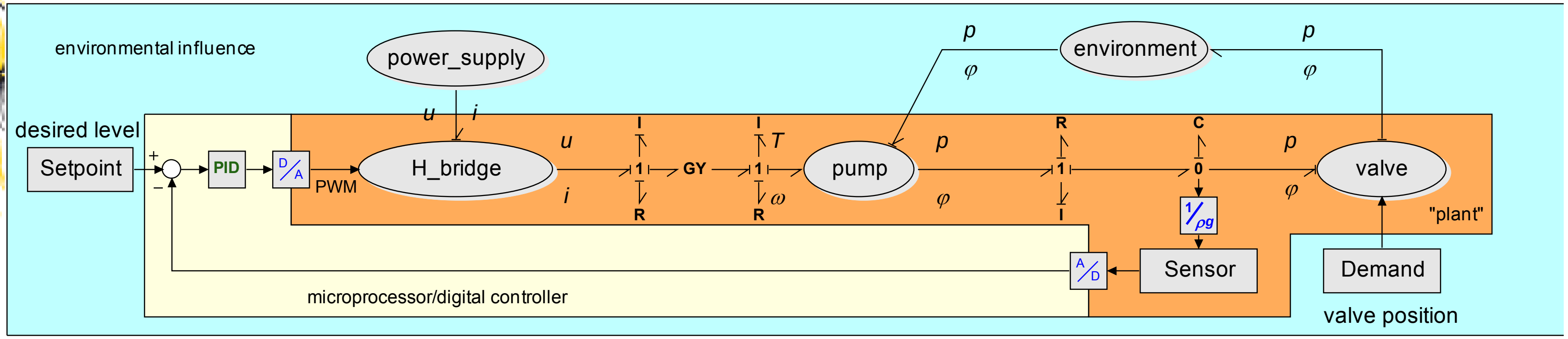
EXAMPLE: FLUID SUPPLY SYSTEM COMPONENT LEVEL



EXAMPLE: FLUID SUPPLY SYSTEM
CONCEPTUAL ELEMENTS



EXAMPLE: FLUID SUPPLY SYSTEM



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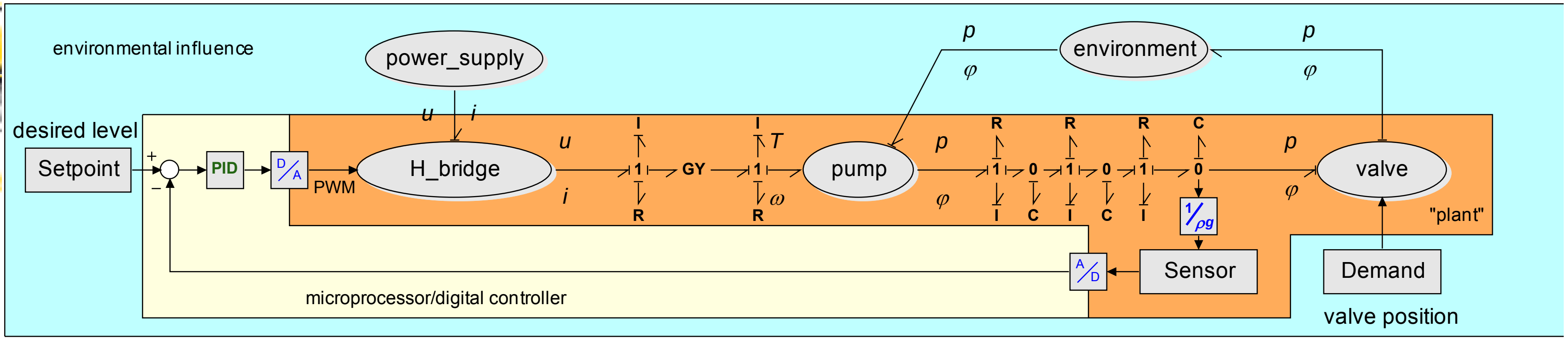


EXAMPLE: ELECTRIC MOTOR

- **Most dominant: power transduction**
- **But also possible:**
  - **Multiport energy storage (magnetic, kinetic, thermal), necessarily reversible (cycle process is always required!), *linear* decomposition results in a transducer and 1-ports**
  - **Separate (conceptual!): irreversible transduction, electrical resistance and mechanical friction**
  - **etc.**

EXAMPLE: FLUID LINE

- **Dominant: fluid resistance**
- **1) If relatively long and narrow: fluid inertia**
  - **Conceptual structure: common flow, summation of pressure drops, not separated in space!**
- **2) Compressibility:**
  - **Several segments (R,I,C)**
  - **Normal modes**
- **3) Compressible fluid, convecting momentum and entropy (also charge, flux,…): conceptual structure**
- **4) Elastic tube wall: mixed boundaries**

TRANSPORT IN ENGINEERING SYSTEMS

- **System boundary: globally Lagrangian (commonly at rest), locally Eulerian (commonly closed)**
- **Tangible subsystem boundaries (components): globally Eulerian (network w.r.t. system boundary), locally Lagrangian (components have fixed neighbors, exceptions require bookkeeping, while major system structure is maintained)**
- ***Conceptual*** **(abstract) subsystem boundaries: structure is based on distinction between basic dynamic behaviors and not based on material or spatial criteria**

‘ENERGY DENSITY’ IMPLIES A FIRST DEGREE HOMOGENEOUS ENERGY

- **Conserved energy has to be a homogeneous function of conserved states:**

$$E(\mathbf{q},m,V): \quad \left(\frac{1}{m}\right)^{n} E\left(\frac{\mathbf{q}}{m},1,\frac{V}{m}\right) = \left(\frac{1}{m}\right)^{n=1} E\left(\frac{\mathbf{q}}{m},1,\frac{V}{m}\right) = \varepsilon_m\left(\frac{\mathbf{q}}{m},v\right)$$

$$E(\mathbf{q},m,V): \quad \left(\frac{1}{V}\right)^{n} E\left(\frac{\mathbf{q}}{V},\frac{m}{V},1\right) = \left(\frac{1}{V}\right)^{n=1} E\left(\frac{\mathbf{q}}{V},\rho,1\right) = \varepsilon_V\left(\frac{\mathbf{q}}{N},\rho\right)$$

- **Convection requires that addition of subsystems means interaction-free addition of extensive states and addition of (extensive) energy:**
- ***n*=1 in principle (if all states are considered!)**

FIRST DEGREE HOMOGENEOUS ENERGY

- **Generalized Gibbs' relation:** $E(\mathbf{q}) = \frac{1}{n}\sum \frac{\partial E}{\partial q_i} q_i \overset{n=1}{=} \sum e_i q_i$

- **First degree homogeneous energy implies zero degree constitutive relations (intensity!):**

$$e_i(\alpha\mathbf{q}) = \frac{\partial E(\alpha\mathbf{q})}{\partial \alpha q_i} = \frac{\alpha\partial E(\mathbf{q})}{\alpha\partial q_i} = \frac{\partial E(\mathbf{q})}{\partial q_i} = \alpha^0 e_i(\mathbf{q})$$

$$\sum_{i=1}^{k} q_i \mathrm{d}\frac{\partial E}{\partial q_i} = \sum_{i=1}^{k} q_i \mathrm{d}e_i = 0$$

k-1 independent **intensities**

- **One-port storage cannot exist *in principle*, unless constant states are considered parameters**

GENERALIZING GIBBS AND GIBBS-DUHEM

$$u = Ts - pv + \sum_{i=1}^{m-1} \mu_i \frac{N_i}{N} + \mu^{tot} \qquad \text{(Gibbs)}$$

$$0 = sdT - vdp + \sum_{i=1}^{m-1} \frac{N_i}{N} d\mu_i + d\mu^{tot} \qquad \text{(Gibbs-Duhem)}$$

$$u = Ts - pv + \sum_{i=1}^{m-1} \mu_i \frac{N_i}{N} + \mu^{tot} + v\frac{\overline{p}}{N} + e_i \frac{q_i}{N} \qquad \text{(Generalized Gibbs)}$$

$$0 = sdT - vdp + \sum_{i=1}^{m-1} \frac{N_i}{N} \mathrm{d}\mu_i + \mathrm{d}\mu^{tot} + \frac{\overline{p}}{N}\mathrm{d}v + \frac{q_i}{N}\mathrm{d}e_i \qquad \text{(Generalized Gibbs-Duhem)}$$

Specific quantities are ‘weighting factors’

CONJUGATE FLOW RELATIONS

$$\left(\frac{\mathrm{d}S}{\mathrm{d}t}\right)_{convected} = \left(\frac{S}{N}\right)\frac{\mathrm{d}N}{\mathrm{d}t}; \quad \left(\frac{\mathrm{d}N_i}{\mathrm{d}t}\right)_{convected} = \left(\frac{N_i}{N}\right)\frac{\mathrm{d}N}{\mathrm{d}t}; \quad \left(\frac{\mathrm{d}V}{\mathrm{d}t}\right)_{convected} = 0!$$

$$\left(\frac{\mathrm{d}q_i}{\mathrm{d}t}\right)_{convected} = \left(\frac{q_i}{N}\right)\frac{\mathrm{d}N}{\mathrm{d}t}; \quad \left(\frac{\mathrm{d}\overline{p}}{\mathrm{d}t}\right)_{convected} = \left(\frac{\overline{p}}{N}\right)\frac{\mathrm{d}N}{\mathrm{d}t}; \quad \left(\frac{\mathrm{d}N_i}{\mathrm{d}t}\right)_{convected} = \left(\frac{N_i}{N}\right)\frac{\mathrm{d}N}{\mathrm{d}t}$$

$$\left(\frac{\mathrm{d}S}{\mathrm{d}t}\right)_{convected} = \left(\frac{S}{N}\right)\frac{\mathrm{d}N}{\mathrm{d}t}; \quad \left(\frac{\mathrm{d}V}{\mathrm{d}t}\right)_{convected} = 0!$$

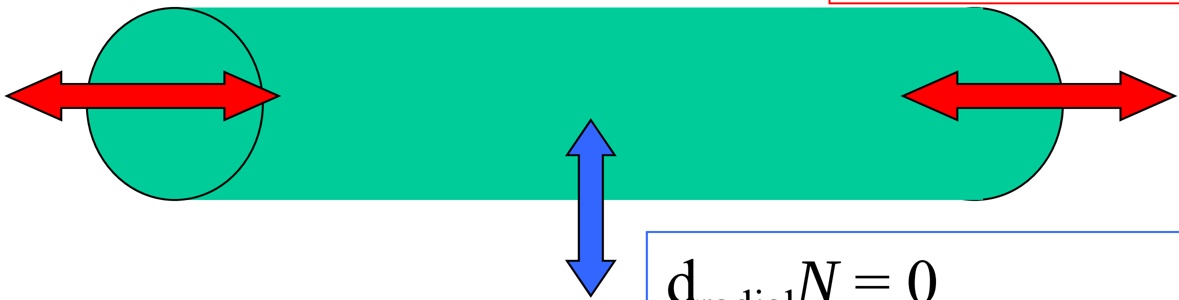
Same specific quantities are ‘weighting factors’

PART OF A TUBE NETWORK

$$\mathrm{d}_{\mathrm{axial}}\, V = 0$$

(V ***not*** *a* ***convected*** *property*)

$$\mathrm{d}_{\mathrm{axial}}\, N \neq 0$$



$$\mathrm{d}_{\mathrm{radial}} N = 0$$

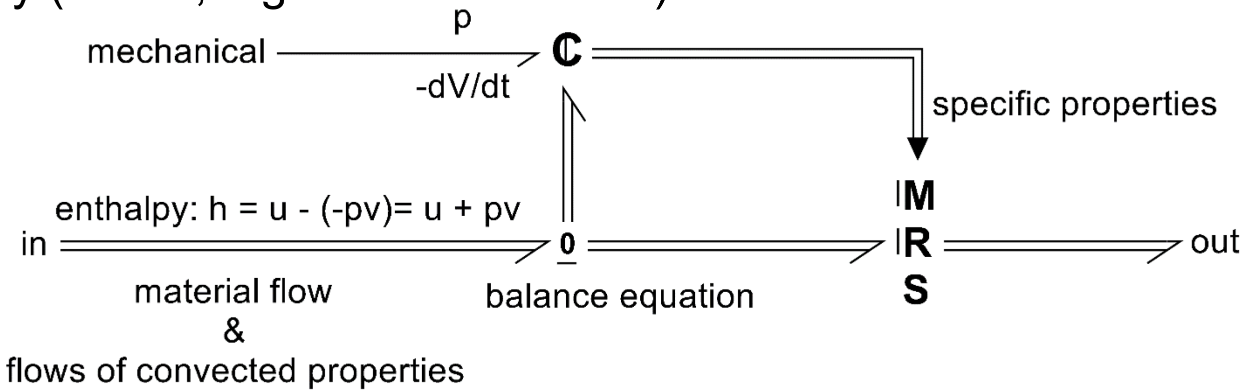
$$\mathrm{d}_{\mathrm{radial}}\, V \neq 0$$

(*flexible tube*, ***local*** *changes*)

GENERIC PICTURE: MASS/MATERIAL FLOW

locally Lagrangian
boundary (d*N* =0; e.g. elastic tube wall)

globally Eulerian
boundary (d*V* =0)

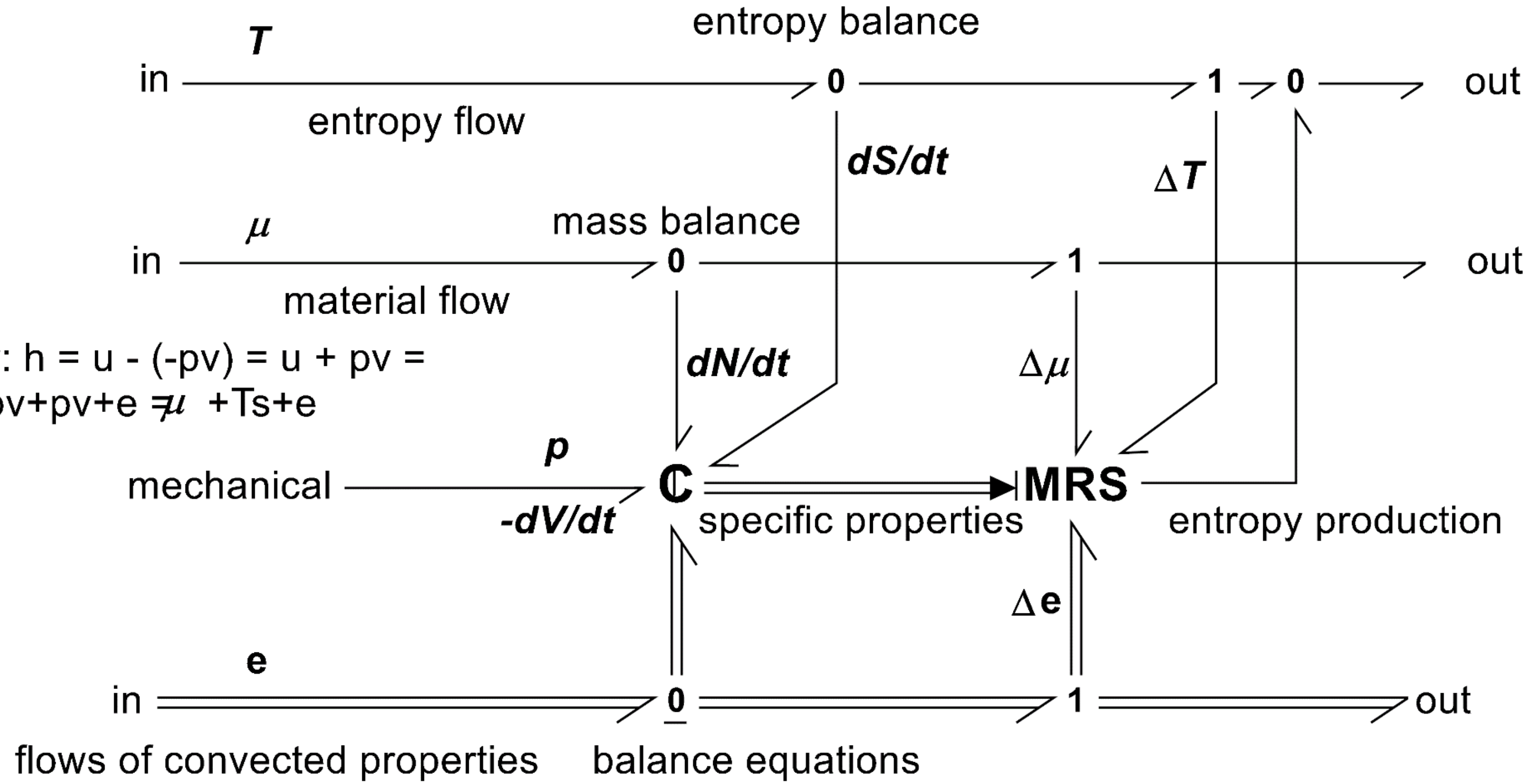


Total energy ‘flow’: $\left(e+pv\right)\frac{dN}{dt}+p\left(-\frac{dV}{dt}\right)=\frac{dE}{dt}$

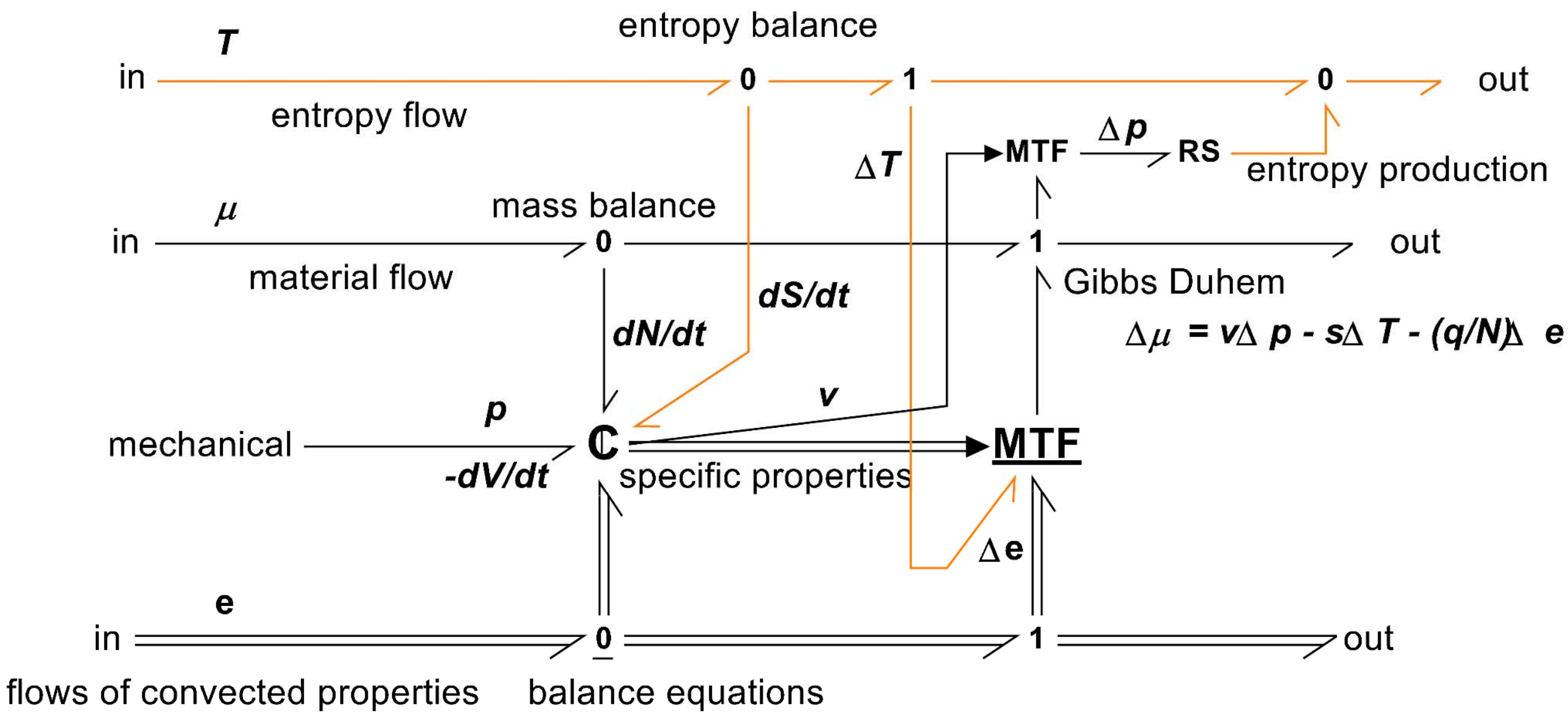
but the specific enthalpy *h* can***not*** serve as an equilibrium-determining variable

GENERIC PICTURE: SPLIT OUT FLOWS

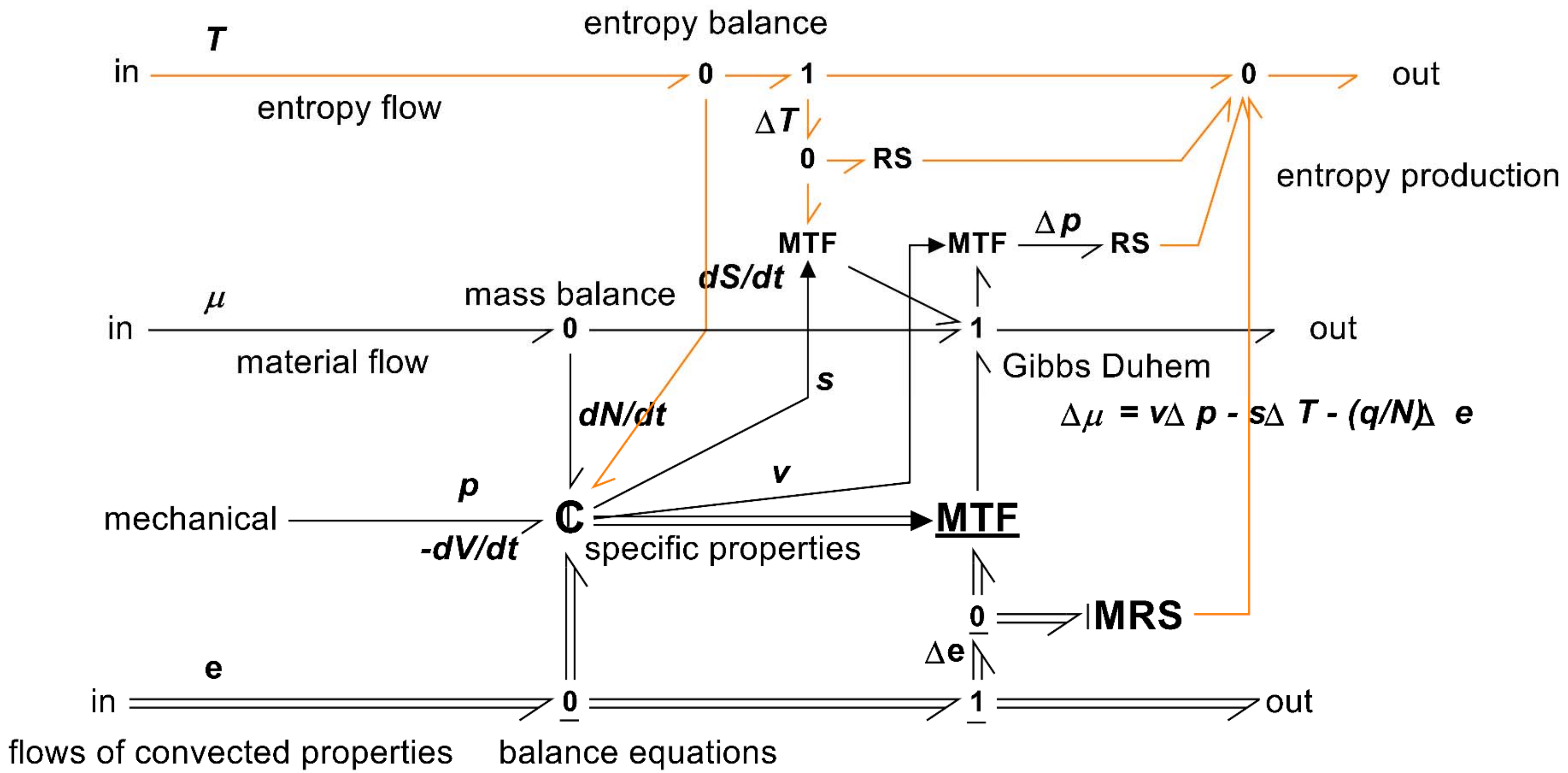
enthalpy: $h = u - (-pv) = u + pv =$
$= \mu + Ts - pv + pv + e = \mu + Ts + e$



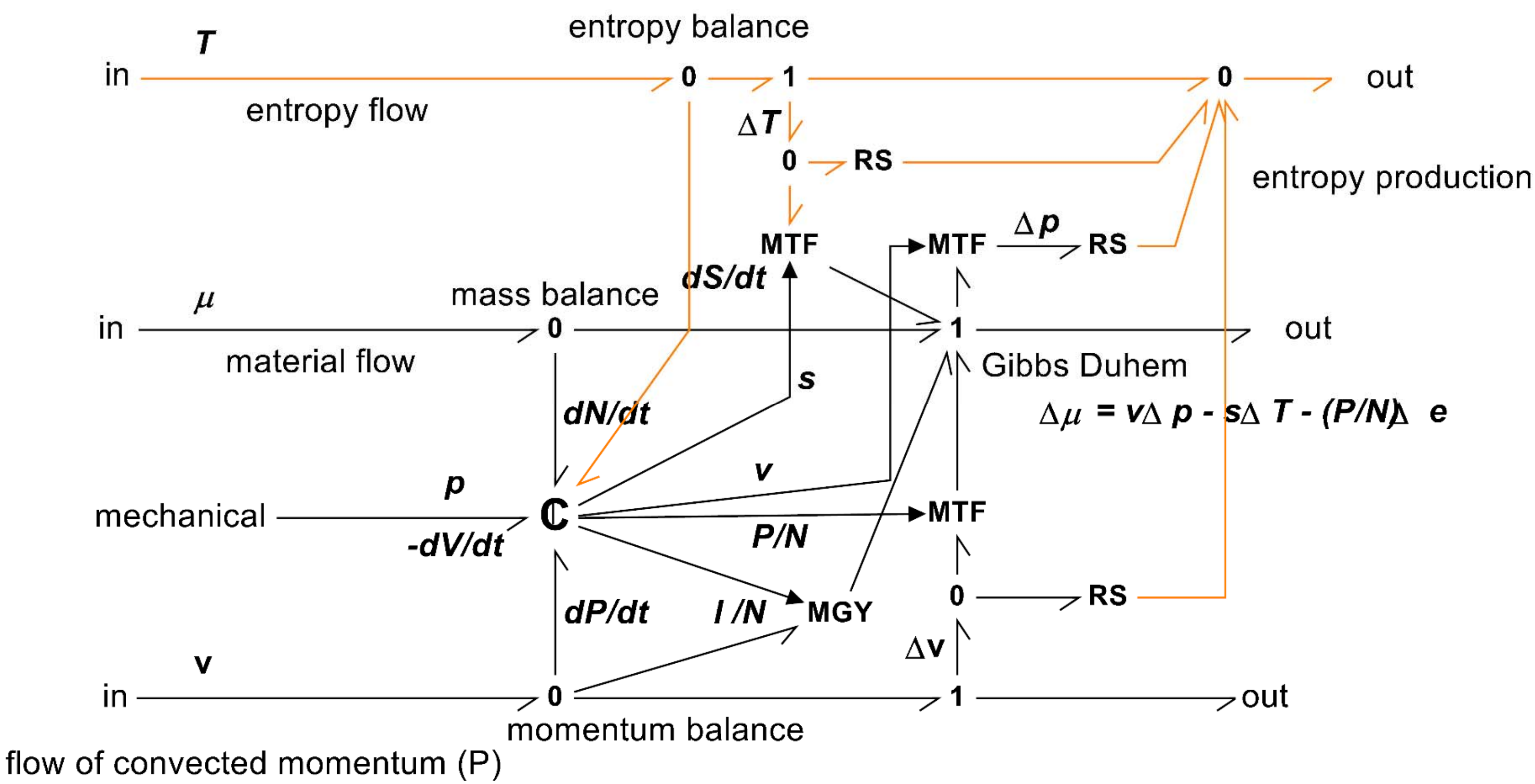
GENERIC PICTURE: NO 'SLIP'



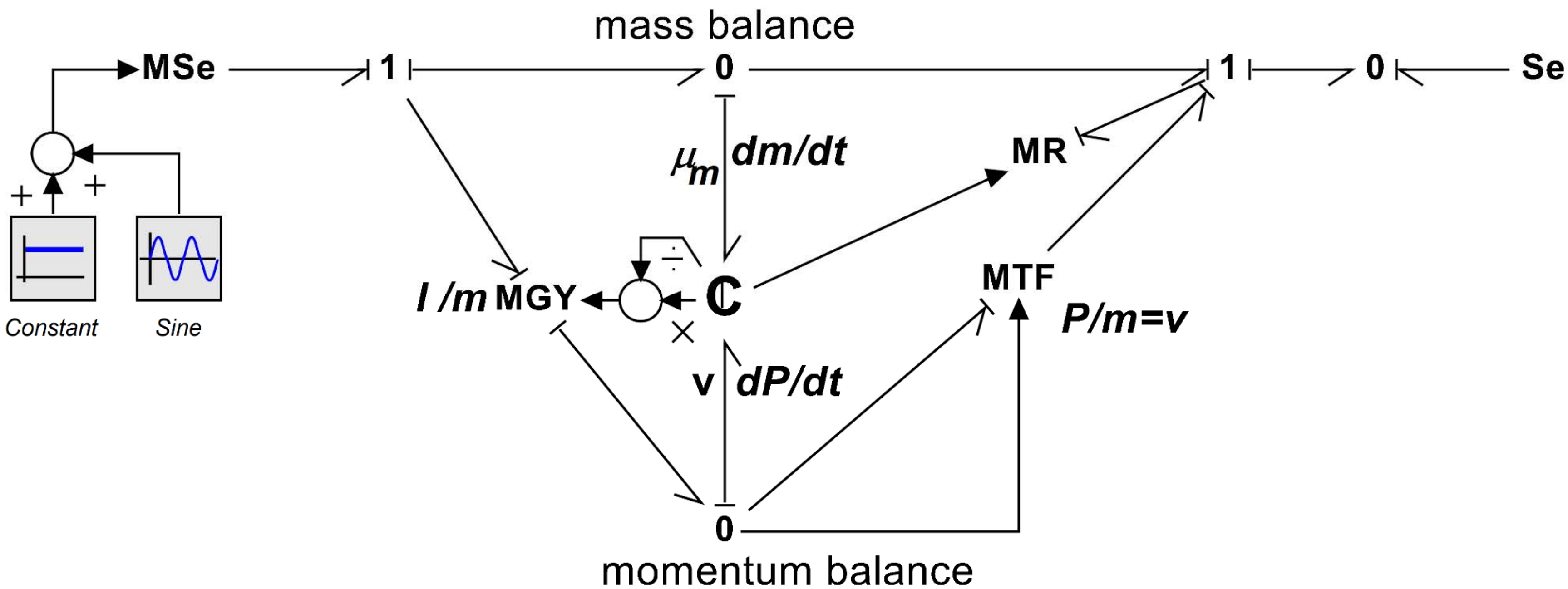
GENERIC PICTURE: WITH 'SLIP' OF CONVECTED PROPERTIES



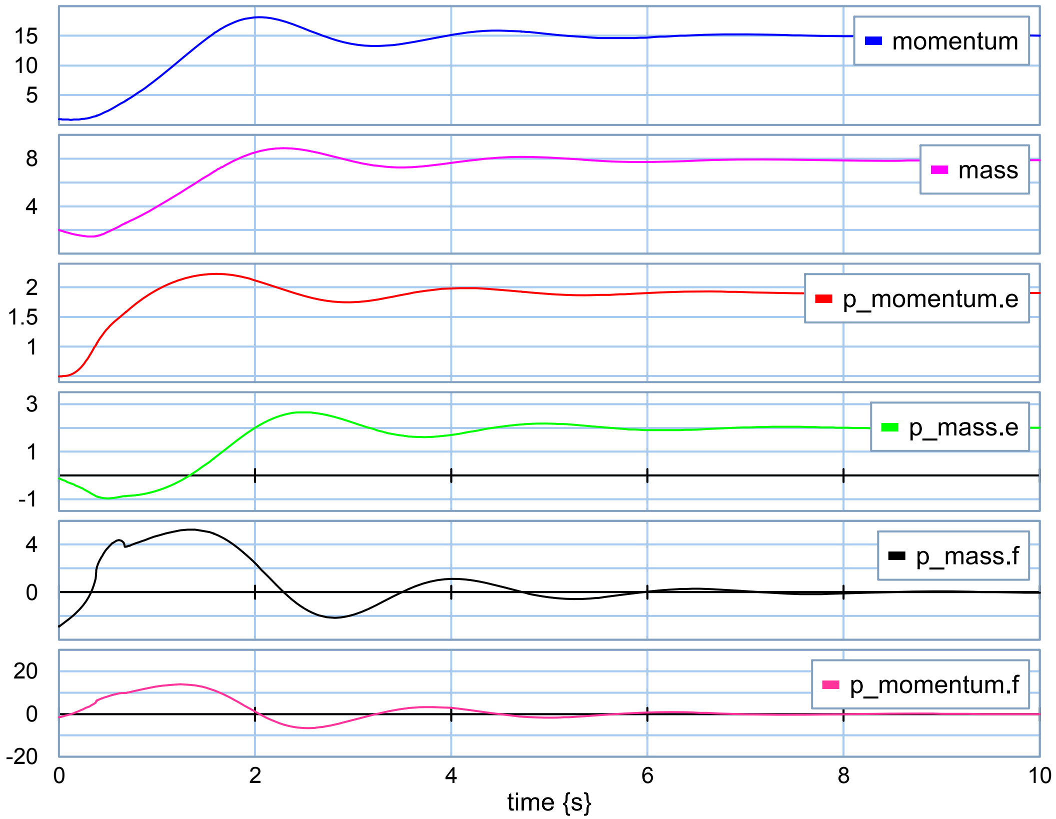
GENERIC PICTURE: MOMENTUM CONVECTION



SIMPLIFIED: MOMENTUM CONVECTION, RIGID TUBE WALL

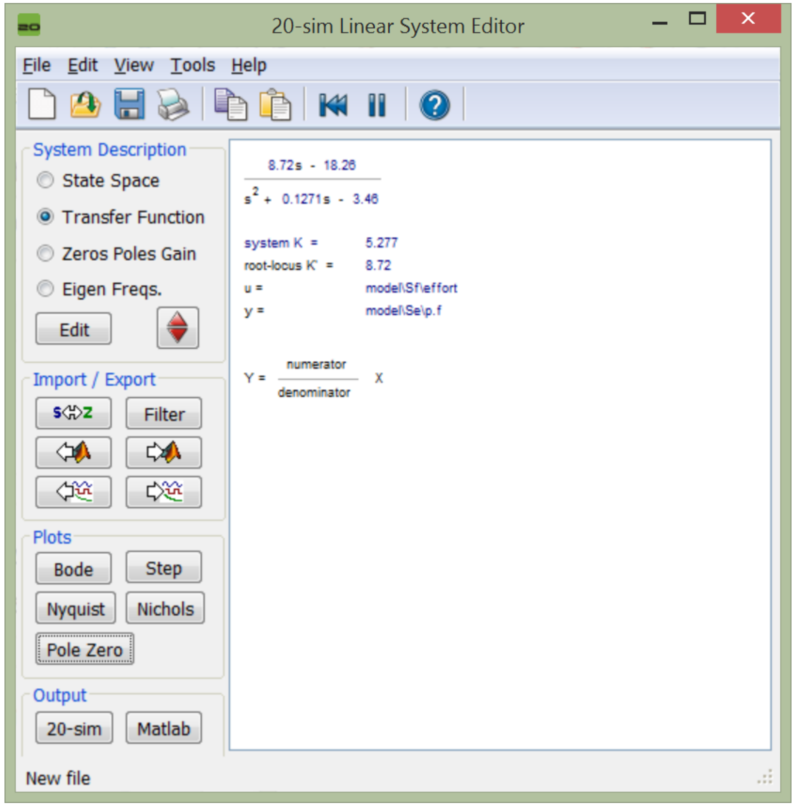


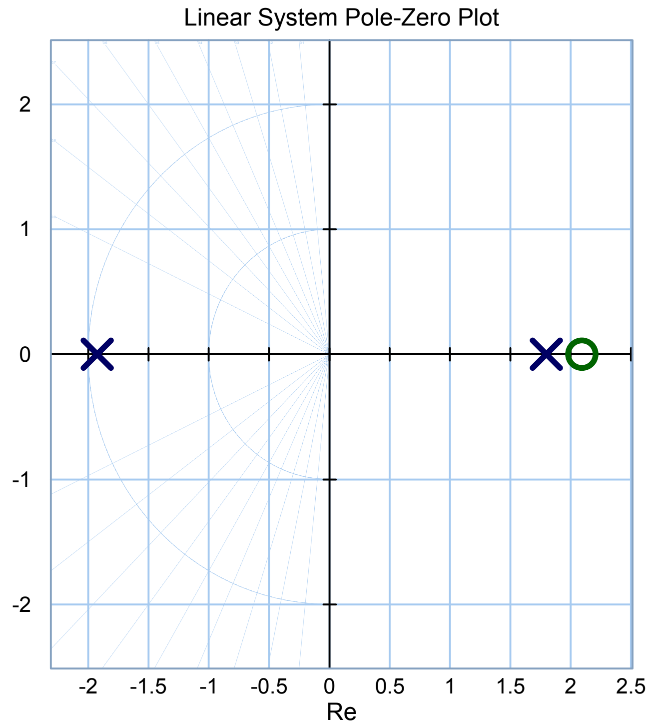
NON-MINIMUM PHASE RESPONSE



Just qualitative, numbers have no meaning!

NON-MINIMUM PHASE RESPONSE





CONCLUSIONS

- separation between *configuration* and *energy* states: more insight
- system boundary definitions may be *mixed*: Eulerian vs Lagrangian
- concept of energy *density* (material of spatial) synonymous with first degree homogeneous energy function of all possible extensive states *in principle*
- energy-based modeling approach:
  - automatically satisfies fundamental principles of physics when all grammar rules are obeyed
  - systematic approach to the dynamic behavior of all properties that may be *convected* in principle (e.g. momentum, electric charge, etc.);
- generalized thermodynamic framework of variables more general than Hamiltonian (generalized mechanical) framework:
  - some domains have no dual storage