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Optimality of Integrated Process Networks

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Abstract— **We introduce a new framework for distributed control and optimization of complex networks. Conservation laws for extensive quantities and the second law of thermodynamics lead to conditions for stability and optimality of the network. We derive a general way of describing interconnections in networks through matrix representations that capture a network's topology using basic principles from electrical engineering methodologies. This shows how the dynamics of independent entities in a network define the objective function of the optimization problem that is simultaneously solved. A generalized version of Tellegen's theorem from electrical circuit theory plays a central role in developing the objective function of the regarded dynamic networks. These results indicate that we can solve optimization problems using dynamical systems, and how the objective function depends on the choice of feedback control and strategies. Examples are presented to illustrate these principles for different types of network connections, both for transient and stationary conditions. We apply the introduced theory to business systems integrated into larger logistic systems.**

Keywords: business systems, process control, flow control, entropy, dissipation, oil production, network theory, irreversible thermodynamics, distributed control, passivity, agents, production optimization, multiphase flow.

I. INTRODUCTION

Information technology has had a tremendous impact on the operation of integrated systems such as logistic supply networks, chemical plants and oil and gas pipeline networks. Such networks can be viewed as complex distributed systems where physics, communication, and computation are integrated so that objectives such as stability and optimality are met simultaneously. Computer technology has enabled fast information exchange and, as a consequence, facilitated fast adaptation to changing conditions [1]. A complete theory for design and operation of such systems is lacking at present. Large scale systems form complex networks in which decentralized parts of the system are highly interconnected both through physical connections and signal flows. The structure of interconnected systems plays a crucial role in their dynamic behavior and has to be well understood to achieve stability and optimality [2].

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A process system can be described as a thermodynamic system where interconnections between process units lead to complex behavior. Thermodynamics is a phenomenological theory and thus, a formal structure which allows to establish relationships between quantities but it cannot account for physical events in detail [3]. Although a thermodynamic description of a process system will not be sufficient to account for all of the complex behavior of the systems, it can give us an idea of how the system evolves over time and show how its behavior depends on the interconnections with the environment. Conservation laws for certain inventories such as energy and mass in process systems confine the system behavior and, combining it with the second law of thermodynamics, we can determine stability and convergence of these systems to a desired steady state. These ideas are particularly useful when applying control and thus influencing the natural evolvement of the system into a desired equilibrium.

The complexity of many process systems arises from the variety of different process subunits and the way they are connected and interact with each other [4]. In general, especially the connections between the subunits lead to complex nonlinear behavior of the total process system. A crucial component in understanding and modeling process systems is therefore to understand how connections between the subunits lead to complex system behavior.

Network theory offers a framework suitable to model and describe the thermodynamics of complex interconnected systems in a modular fashion [5]. The purpose of network theory in this application to process systems is therefore to provide an organizational framework for treating complex process systems. The techniques we develop here are particularly suitable for the description of process systems due to the nonlinear dynamics of individual processes, the organizational complexity of the entire system and the intricacy of the resulting detailed mathematical equations [6].

The formalism of network theory has been particularly successful for the control and modeling of dynamics systems in electrical engineering. Classically, electrical circuit theory is not considered an application of non-equilibrium thermodynamics. Nevertheless, electrical circuits are typical irreversible thermodynamic systems. The formalism developed in electrical circuit theory can however easily be extended to general thermodynamic systems [5], [6]. In particular the application to complex biological systems has been successfully carried out [7], [8]. Network theory brings thermodynamics a degree of mathematical rigor and allows to unify ideas from non-equilibrium thermodynamics, dynamic system theory and control. If we look at the mathematical models of many dynamic physical systems, we can typically identify two mathematical structures underlying most physical models. There is the kinematic structure which addresses the topology of the system and a dynamical structure [7]. The connectivity properties of the system describe the physical processes where the dynamical structure defines the relationships between the state variables to characterize the system.

In this paper, we propose to analyze complex dynamical systems in terms of their network character. We develop a theoretical framework for distributed control and optimization of such networks by combining ideas from thermodynamics, electrical circuit theory, and mathematical system theory.

II. PROCESS NETWORKS

Let Σ be a convex sub-set of $\mathbb{R}^n_+$ and let $Z = (Z_1, ..., Z_n)$ represent an arbitrary point. The vector Z can be regarded as the inventory of n different properties of the system $\mathscr{P}$. We distinguish between two types of inputs and outputs. The signals, y and u, represent measured outputs and control inputs. The vectors f_j can be thought of as physical flows which connect the system to other process systems or the environment. The two-port representation allows different algebraic structures for the representation of physical flows and signals. The state of the process system evolves according to the conservation laws

$$\frac{dZ}{dt} = p(Z) + \sum_{i=1}^{m} f_i(u, Z, d), \; Z(0) = Z_0 \quad (1)$$

$$y = h(Z) \quad (2)$$

The vector Z_0 is the initial condition, $p(Z)$ defines the rate of generation of Z, the vectors $f_i(u,Z,d)$, $i = 1, ..., n$ denote flows. The flows may depend on control signals u, the state as well as external signals d which represent boundary conditions. The vector y denotes the measurements. We now define a class of $\mathbb{C}_1$ functions $\varepsilon(Z) : \Sigma \longmapsto \mathbb{R}_+$ called extensions. An extension is said to be conserved if its rate of production equals zero. It is dissipative if its production is less or equal to zero and it satisfies the Clausius Planck inequality if its rate of production is greater or equal to zero [3]. Mass and energy are examples of extensions that satisfy all these properties. The entropy of classical thermodynamics satisfies the Clausius Planck inequality. The extensions used in passivity theory are called storage or dissipation functions and they satisfy the dissipation inequality.

Definition 1: A system $\mathscr{P}$ with conservation laws (1) is called a process system if there exist extensions $S(Z)$ and $E(Z)$ so that

1) S(Z) is concave in Z.
2) S(Z) is positively homogeneous of degree one in Z.
3) E(Z) is conserved and $T = \frac{\partial E}{\partial S}$.

The function $S(Z)$ is called the entropy, the function $E(Z)$ is called the energy and T is called the temperature.

We can now define a network of processes in which each node can be a process system:

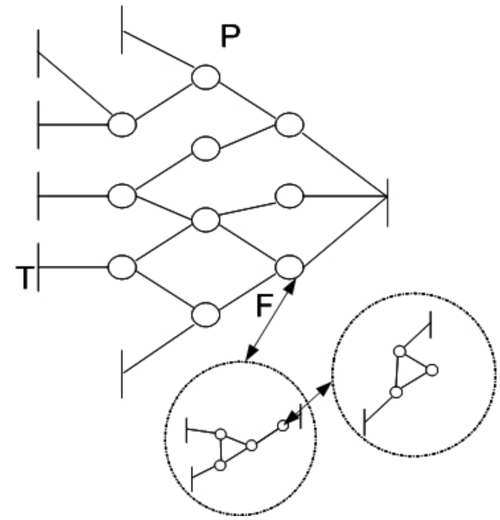

Fig. 1. Graphical network representation: Topological structure of a network consisting of nodes, terminals, and flows. Nodes can contain subgraphs and give rise to a hierarchical multiscale structure.

Definition 2: A network of vertices $P_i, i = 1, ..., n_p, n_p + 1, ..., n_t$ consisting of nodes and terminals interconnected through edges $F_i, i = 1, ..., n_f$ with topology defined by the graph

$$\mathbf{G} = (\mathbf{F}, \mathbf{P})$$

is called a network if:

1) We can uniquely define the state of the network through the state of the nodes Z_i
2) Conservation laws for extensive quantities Z_i hold.
3) The first order homogeneous function $S(Z_i) = Z_i w_i$ defines a concave storage function at each node P_i. The potential at the nodes is defined as $w_i = \frac{\partial S_i}{\partial Z_i}$.

A representation to graphically display the topology of an arbitrary network is given in Fig. 1. We follow the graph notation by Desoer [9] according to the following definition:

Definition 3: The $n_t \times n_f$ matrix $\mathbf{A_a}$ is called node-to-branch incidence matrix for the matrix elements a_{ij} being

$$a_{ij} = \begin{cases} 1, & \text{if flow } j \text{ leaves node } i \\ -1, & \text{if flow } j \text{ enters node } i \\ 0, & \text{if flow } j \text{ is not incident with node } i \end{cases}$$

A reference or datum node P_0 is introduced to represent the environment and connected to all dynamic nodes and terminals. The $(n_t - 1) \times n_f$ matrix A, where the row that contains the elements a_{0j} of the reference node P_0 is eliminated, is called reduced incidence matrix.

The incidence matrix A_a and the reduced incident matrix have same rank $r = n_t - 1$ and, therefore, the row of the reference node is a linear combination of the preceding rows [9]. We can use the matrix representation of the network to formulate the conservation laws for the nodes:

$$\mathbf{AF} = \mathbf{0} \quad (3)$$

where $\mathbf{F^T} = [\frac{dZ_1}{dt}, \frac{dZ_2}{dt}, ..., \frac{dZ_t}{dt}, f_{12}, f_{13}...f_{n_{t-1},n_t}, p_1, ..., p_t]$. The flows f_{ij} represent connections between two nodes i.e. f_{ij} connects node i to node j, p_i denotes sources or sinks. Equation (3) corresponds to Kirchhoff's current law (KCL) of electrical circuit theory in a generalized form.

We can define a change in potential from node i to j as $W_{ij} = w_i - w_j$. The potential difference W_{ij} acts as a driving force which induces flow between nodes i and j. The flows are connected to the potential differences through constitutive relationships of the form

$$\mathbf{F} = \mathbf{K}(\mathbf{u})\mathbf{W} \tag{4}$$

where u is an optimization or control parameter and $\mathbf{K}(\mathbf{u})$ is a matrix function.

From our definition of potentials, we conclude that potential differences around any closed loop or mesh in the network for any given mesh inside the network [10] add up to zero. Using the matrix notation introduced in Definition 3, we denote the mesh equations as

$$\mathbf{W} = \mathbf{A^T w} \tag{5}$$

where we use the transpose of the reduced incident matrix $\mathbf{A}$ [9]. The matrix equation (5) correspond to a generalized Kirchhoff's voltage law (KVL) of electrical circuit theory. In order to determine the state of the network at any given point in time, it is necessary to model the connection structure through the incident matrix and pose the constitutive relations between the potentials W and flows F for each branch in the network. In addition, we have to supply one boundary condition for each terminal in the network. In the dynamic case, it is necessary to define initial conditons for the inventories $Z_i(0)$ for every dynamic node.

III. THE TELLEGEN THEOREM FOR PROCESS NETWORKS

In this section, we develop a theorem that is only based on the topological properties of the process network. The so called Tellegen theorem plays an important role in deriving an objective function for network optimization problems.

Theorem 1: For any two networks denoted by the superscripts a and b that follow Definition 1 with the same topology, i.e. same reduced incidence matrix $\mathbf{A}$,

$$\sum_{i=1}^{n_f} F_i^a W_i^b = \sum_{i=1}^{n_f} F_i^b W_i^a = 0 \tag{6}$$

Proof:

$$\sum_{i=1}^{n_b} F_i^a W_i^b = (\mathbf{W^b})^\mathbf{T}\mathbf{F^a} \tag{7}$$

using KVL (5)

$$= (\mathbf{A^T w^b})^\mathbf{T}\mathbf{F^a} \tag{8}$$

$$= ((\mathbf{w^b})^\mathbf{T}\mathbf{A})\mathbf{F^a} \tag{9}$$

$$= (\mathbf{w^b})^\mathbf{T}\mathbf{A}\mathbf{F^a} = \mathbf{0} \tag{10}$$

since $\mathbf{AF^a} = \mathbf{0}$ using KCL (3).

■

The Tellegen theorem holds for any two networks with the same topology even if they consist of different network elements. It is also valid for any network being in two different states and holds true for time evolving networks. In case, we regard only one network, it reduces to an energy balance. The constitutive equations (4) may be nonlinear or linear, discrete or continuous, passive or active, and the network may have single or multiple steady states.

IV. PASSIVITY OF PROCESS NETWORKS

Passivity theory offers a physics based mathematical framework for the analysis of stability and control of networked process systems with nonlinear dynamics. According to the passivity concept, all states of the system can be stabilized, if the total energy and mass of the system are bounded. To prove passivity for the framework here, we have to find a storage function according to the following definition from [10]:

Definition 4: A process network is said to be dissipative with respect to the supply rate $\phi(y,u)$ if there exists a storage function $V(Z)$ so that for all $t \geq 0$, all initial conditions and all controls

$$0 \leq V(Z(t)) \leq V(0) + \int_0^t \phi(y,u)ds \tag{11}$$

In order to find controls for the system, we have to identify passive input-output pairs of extensive and intensive variables for the network as given by y and u for the supply rate $\phi(y,u)$ in (11 which correspond to the terminal potential and flows for the pipeline network. For the case in which we can determine passive properties of the regarded networked process system, the system naturally converges to a state in which the entropy production is a minimum [10].

Passivity follows directly from the properties of the flow connections and the production at the nodes.

Definition 5: A connection is said to be positive if there exists constant $\beta \geq 0$ so that

$$(W^1 - W^2)^T(F^1 - F^2) \geq \beta \left\| W^1 - W^2 \right\|$$

The connection is strictly positive if $\beta > 0$.

W^i, F^i are the potential differences between any two nodes and the connecting flows at two arbitrary states i of the network.

Theorem 2: A process system P is passive if the flows are positive and $(\mathrm{p}^1 - p^2)^T(w^1 - w^2) \geq 0$

Proof: The proof is given in [10]. ■

V. OPTIMALITY OF PROCESS NETWORKS

Based on the Tellegen theorem as an objective function, we can propose an optimization problem that allows us to find the steady state of a dynamic process network.

Theorem 3: Consider a process network G as defined in Definition 1 with given passive constitutive equations and boundary conditions for each terminal. The solution ($\frac{dZ_i}{dt} = 0$) for the network with equations (3) and (5) and the constitutive equations (4) is given by solving the following optimization problem:

$$\min_{\mathbf{F} \text{ or } \mathbf{W}} \quad \sum_{i=1}^{n_f} F_i W_i \tag{12}$$

$$s.t. \quad \mathbf{W} = \mathbf{A^T w} \text{ or } \mathbf{AF} = \mathbf{0} \tag{13}$$

$$\mathbf{F} = \mathbf{KW} \tag{14}$$

$$\mathbf{F_T} = \mathbf{F_T}(t) \text{ or } \mathbf{W_T} = \mathbf{W_T}(t) \tag{15}$$

Proof:

Lagrange function:

$$L(\mathbf{F}, \mathbf{W}, \mathbf{w}, \lambda, \mu) = \mathbf{W^T F} + \lambda^\mathbf{T}(\mathbf{W} - \mathbf{A^T w}) + \mu^\mathbf{T}(\mathbf{F} - \mathbf{KW}) \tag{16}$$

Karush-Kuhn-Tucker conditions:

$$\frac{\partial L}{\partial \mathbf{W}} = \mathbf{F} + \lambda - \mathbf{K}\mu = \mathbf{0} \tag{17}$$

$$\frac{\partial L}{\partial \mathbf{F}} = \mathbf{W} + \mu = \mathbf{0} \tag{18}$$

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{A}\lambda = \mathbf{0} \tag{19}$$

$$\frac{\partial L}{\partial \lambda} = \mathbf{W} - \mathbf{A^T w} = \mathbf{0} \tag{20}$$

$$\frac{\partial L}{\partial \mu} = \mathbf{F} - \mathbf{KW} = \mathbf{0} \tag{21}$$

Solving (18) for μ and substituting in (17), then solving (17) for λ and substituting in (19) gives

$$\mathbf{A}(\mathbf{F} + \mathbf{KW})) = \mathbf{0}$$

using the constitutive equations (4) to substitute **KW** results in:

$$\mathbf{AF} = \mathbf{0}$$

which is the Kirchhoff current law.

■

The objective function is a measure for dissipation of the storage variable over time. We conclude that the steady state of a passive network minimizes the dissipated power subject to the constraints imposed by the constitutive equations, topology, and boundary conditions, i.e. terminal connections.

So far, we performed a node analysis and formulated KVL and KCL in form of the nodal incident matrix. The analysis can as well be performed and the topology captured using a mesh analysis, where the inner meshes are forming the incident matrix M and the outer mesh is redundant and linearly dependent.

The optimization problem can be formulated as follows:

$$\min_{\mathbf{F} \text{ or } \mathbf{W}} \quad \sum_{i=1}^{n_f} F_i W_i \tag{22}$$

$$s.t. \quad \mathbf{F} = \mathbf{M^T f} \text{ or } \mathbf{MW} = \mathbf{0} \tag{23}$$

$$\mathbf{F} = \mathbf{KW} \tag{24}$$

$$\mathbf{W_T} = \mathbf{W_T}(t) \text{ or } \mathbf{F_T} = \mathbf{F_T}(t) \tag{25}$$

Proof:

The proof works analogously to the node analysis formulation and results in the derivation of KVL for mesh analysis.

$$\mathbf{MW} = \mathbf{0}$$

The findings in this section indicate that we have a dual formulation given for the optimization problem. As already shown for the Tellegen theorem, flows and potentials are orthogonal spaces and duality of the matrix representation and optimization problem are an important property of our class of networks.

VI. APPLICATION TO BUSINESS SYSTEMS

In this section, we apply the network theory developed in the previous section to model financial, material and service flows in business systems. Decision making in a business system has to be understood as a multiobjective optimization problem [11], [12] on different time and hierarchical scales. Business organizations can be regarded as complex networks in which a combination of centralized and decentralized decision making aims to optmize a business' performance [13]. Regardless of the complexity, a business' objective to maximize its profit and as a consequence its total value is often implemented through very simple decentralized management policies that lead to self-optimizing structures using key indicators such as the Net Present Value or the Return on Investment [14]. We attempt to point out how this modeling approach can support understanding the network character of business systems, help explore self-optimizing structures, and develop optimization and control policies for complex and highly interconnected business systems [12].

We define a network of activities of a business organization according to Definition 1. At the vertices of the business network activities take place in which material, cash or liabilities can be stored, routed, or transformed as depicted in Fig. 2. The connections between the vertices represent material or financial flows. The terminals on the left hand side are connections to suppliers, the ones on the right hand side represent the costumers which connect the business to economic markets.

For our discussion, it is convenient to define the following extensive variables when we develop an abstract framework for business decision making. These variables describe the assets

$$a = \begin{cases} a^{current} - \text{ current assets (inventory } I \text{ and cash } c) \\ a^{fixed} - \text{ fixed assets (buildings equipment)} \\ a^{other} - \text{ other assets (patents, market position)} \end{cases}$$

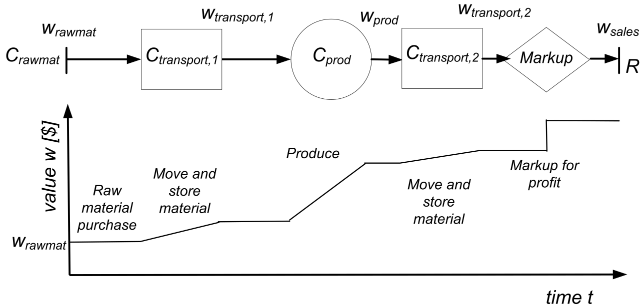

Fig. 2. The value chain tracks how process operations add value to goods as they move through the production system. The last section includes the price markup as a value added step.

and liabilities

$$l = \begin{cases} l^{current} - \text{ short term liabilities (outstanding bills)} \\ l^{longterm} - \text{ long term liabilitites (loans, mortgages)} \end{cases}$$

Material, service and cash flows entering and leaving a node are conserved. Forming a vector of all assets **a** and liabilities **l** for each node, the inventories of assets and liabilities for all vertices $\mathbf{v}^T = (\mathbf{a_1}^T, \mathbf{l_1}^T, \mathbf{a_2}^T, \mathbf{l_2}^T, ..., \mathbf{a_{n_p}}^T, \mathbf{l_{n_p}}^T)$ determine the state of the dynamic system under consideration that the flows determine how assets and liabilities are re-allocated throughout the business organization.

The dynamic system consists of input-output variables i.e. the incoming and outgoing flows of assets and liabilities.

$$\frac{d\mathbf{v}}{dt} = \phi(\mathbf{u}, \mathbf{t}) + \mathbf{p} \tag{26}$$

(26) corresponds to the Kirchhoff current law. We now define potentials in form of prices or values w at the nodes in the network according to the network theory presented in the last sections. In order to introduce potentials, we need to define an appropriate storage function for business systems. Herefore, the storage function $E(v)$ is used to capture the total value of the business

$$E = A - L \tag{27}$$

E formally corresponds to the shareholder or owner equity (net worth) of a business. We also define the functions value of all assets A and value of all liabilities L

$$A = \sum_{i}^{N^assets} a_i w_{a,i}, \text{value of assets [Value]} \tag{28}$$

$$L = \sum_{i}^{N^assets} l_i w_{l,i}, \text{ liabilities [Value]} \tag{29}$$

$$\tag{30}$$

After defining an appropriate storage function for the business network, we can now derive potentials w for each node in the network through partial derivatives.

The companies value is then defined through the net worth or owner's/shareholder equity $E(v)$. A companies objective is to maximize its total value over time. An increase of the value can be achieved through a positive cost/profit balance of all the activities. The profit of an activity is calculated so that

$$P(t) = \int_{t}^{t+T} (R - C) ds \tag{31}$$

where T is the reporting period, R is the rate of income and from sales and C is the rate of cost. The difference $R - C$ is called rate of accounting earning. The activity costs include transportation, storage, manufacture (assembly), and purchase. By differentiating the expression above, we obtain the differential balance

$$\frac{dP}{dt} = R - C \tag{32}$$

(32) corresponds to the Tellegen theorem previously introduced through (6) for one network. The cost rates through transportation, manufacture and storage corresponds to dissipative elements of our general network definition. The earnings through sales R and cost through purchase can be regarded as in/outflux of value through terminals. Analogously to the optimization problem in the last section, a business organization intends to maximize the rate of accounting earnings $R - C$ to achieve maximum profit. This can be achieved through minimizing the total rate of cost of the network which corresponds to the optimization problem posed in the last section.

VII. CONCLUSIONS AND FUTURE WORKS

A. Conclusions

A modeling framework has been developed to describe complex process networks. The framework is based largely on fundamental ideas from thermodynamics, including the use of a storage function, as well as flows or production of extensive variables based on potentials or potential differences. The developed framework is derived through a matrix representation of the flows and nodes and allows a compact formulation of basic network properties. Optimality of this class of process networks was demonstrated by formulating the optimization problem that is solved for a dynamic network converging into steady state. The Tellegen theorem serves as an objective function in this framework. We have shown that the used modeling framework can be applied to business systems represented as value added networks.

B. Future Works

Future work will focus on developing a framework to integrate transformation of extensive quantities in the topology of the network. The decentralized optimization problem will be extended for transient conditions. This implies showing that the solutions of the dynamical system solve an optimal control problem and that the state trajectory of the network is determined by solving Euler-Lagrange equations for the problem at hand. Further research will include uncertainty, stochastic processes, and discounting, in particular in the context of modeling business organizations [12]. One goal of this work is to relate decentralized decision making using passivity based control in complex networks to the method of Lagrangian decomposition for solving large scale optimization problems.

We further explore the developed theory for a petroleum production optimization problem for oil reservoir management in the North Sea. The work focuses on applying network theory to integrate the given offshore pipeline network into economic markets and perform simulations of distributed optimization on particular clusters of the regarded platform.

The integrated network will be analyzed using averaging and decomposition methods to investigate the system on different hierarchical levels and time scales, developing a decentralized control network, smart agents [15], [16], and decision making policies based on passitivity theory. The applied decentralized control will be developed to implement self-optimizing structures in the pipeline system. This contributes to the optimization of the offshore pipeline network on a global level for changing operating conditions.

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