

Thermodynamic Modeling, Energy Equipartition, and Nonconservation of Entropy for Discrete-Time Dynamical Systems

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Abstract—In this paper we develop thermodynamic models for discrete-time large-scale dynamical systems. Specifically, using compartmental dynamical system theory, we develop energy flow models possessing energy conservation, energy equipartition, temperature equipartition, and entropy nonconservation principles for discrete-time, large-scale dynamical systems. Furthermore, we introduce a *new* and dual notion to entropy, namely, *ectropy*, as a measure of the tendency of a dynamical system to do useful work and grow more organized, and show that conservation of energy in an isolated thermodynamic system necessarily leads to nonconservation of ectropy and entropy. In addition, using the system ectropy as a Lyapunov function candidate we show that our discrete-time, large-scale thermodynamic energy flow model has convergent trajectories to Lyapunov stable equilibria determined by the system initial subsystem energies.

I. INTRODUCTION

Thermodynamic principles have been repeatedly used in continuous-time dynamical system theory as well as information theory for developing models that capture the exchange of nonnegative quantities (e.g., mass and energy) between coupled subsystems (see [1] and the numerous references therein). In particular, conservation laws (e.g., mass and energy) are used to capture the exchange of material between coupled macroscopic subsystems known as compartments. Each compartment is assumed to be kinetically homogeneous, that is, any material entering the compartment is instantaneously mixed with the material in the compartment. These models are known as *compartmental* models and are widespread in engineering systems as well as biological and ecological sciences [2]–[4]. Even though the compartmental models developed in the literature are based on the first law of thermodynamics involving conservation of energy principles, they do not tell us whether any particular process can actually occur; that is, they do not address the second law of thermodynamics involving entropy notions in the energy flow between subsystems.

The goal of the present paper is directed toward developing nonlinear discrete-time compartmental models that are consistent with thermodynamic principles. Specifically, since thermodynamic models are concerned with energy flow among subsystems, we develop a nonlinear compartmental dynamical system model that is characterized by energy conservation laws capturing the exchange of energy between coupled macroscopic subsystems. Furthermore, using graph theoretic notions we state three thermodynamic axioms consistent with the zeroth and second laws of

thermodynamics that ensure that our large-scale dynamical system model gives rise to a thermodynamically consistent energy flow model. Specifically, using a large-scale dynamical systems theory perspective, we show that our compartmental dynamical system model leads to a precise formulation of the equivalence between work energy and heat in a large-scale dynamical system.

Next, we give a deterministic definition of entropy for a large-scale dynamical system that is consistent with the classical thermodynamic definition of entropy and show that it satisfies a Clausius-type inequality leading to the law of entropy nonconservation. Furthermore, we introduce a *new* and dual notion to entropy, namely, *ectropy*, as a measure of the tendency of a large-scale dynamical system to do useful work and grow more organized, and show that conservation of energy in an isolated thermodynamically consistent system necessarily leads to nonconservation of ectropy and entropy. Then, using the system ectropy as a Lyapunov function candidate we show that our thermodynamically consistent large-scale nonlinear dynamical system model possesses a continuum of equilibria and is *semistable*, that is, it has convergent subsystem energies to Lyapunov stable energy equilibria determined by the large-scale system initial subsystem energies. In addition, we show that the steady-state distribution of the large-scale system energies is uniform leading to system energy equipartitioning corresponding to a minimum ectropy and a maximum entropy equilibrium state. Finally, we note that the proofs of the results in this paper are similar to the proofs given in [1] and hence are omitted. For details of the proofs see [5].

II. MATHEMATICAL PRELIMINARIES

In this section we introduce notation, several definitions, and some key results needed for developing the main results of this paper. Let \mathbb{R} denote the set of real numbers, \mathbb{Z}_+ denote the set of nonnegative integers, \mathbb{R}^n denote the set of $n \times 1$ column vectors, $(\cdot)^T$ denote transpose, and let I_n or I denote the $n \times n$ identity matrix. For $v \in \mathbb{R}^q$ we write $v \geq 0$ (respectively, $v \gg 0$) to indicate that every component of v is nonnegative (respectively, positive). In this case we say that v is *nonnegative* or *positive*, respectively.

Let $\overline{\mathbb{R}}_+^q$ and \mathbb{R}_+^q denote the nonnegative and positive orthants of \mathbb{R}^q , that is, if $v \in \mathbb{R}^q$, then $v \in \overline{\mathbb{R}}_+^q$ and $v \in \mathbb{R}_+^q$ are equivalent, respectively, to $v \geq 0$ and $v \gg 0$. Finally, we write $\Delta V(x(k))$ for $V(x(k+1)) - V(x(k))$.

The following definition introduces the notion of nonnegative functions [6].

This research was supported in part by AFOSR under Grant F49620-03-1-0178 and NSF under Grant ECS-0133038.

Definition 2.1: Let $w = [w_1, \dots, w_q]^T : \mathcal{V} \rightarrow \mathbb{R}^q$, where \mathcal{V} is an open subset of \mathbb{R}^q that contains $\overline{\mathbb{R}}_+^q$. Then w is *nonnegative* if $w_i(r) \geq 0$ for all $i = 1, \dots, q$ and $r \in \overline{\mathbb{R}}_+^q$.

Proposition 2.1 ([6]): Suppose $\overline{\mathbb{R}}_+^q \subset \mathcal{V}$. Then $\overline{\mathbb{R}}_+^q$ is an invariant set with respect to

$$r(k+1) = w(r(k)), \quad r(0) = r_0, \quad k \in \overline{\mathbb{Z}}_+, \quad (1)$$

if and only if $w : \mathcal{V} \rightarrow \mathbb{R}^q$ is nonnegative.

The following definition introduces several types of stability for the discrete-time *nonnegative* dynamical system (1).

Definition 2.2: The equilibrium solution $r(k) \equiv r_e$ of (1) is *Lyapunov stable* if, for every $\varepsilon > 0$, there exists $\delta = \delta(\varepsilon) > 0$ such that if $r_0 \in \mathcal{B}_\delta(r_e) \cap \overline{\mathbb{R}}_+^q$, then $r(k) \in \mathcal{B}_\varepsilon(r_e) \cap \overline{\mathbb{R}}_+^q$, $k \in \overline{\mathbb{Z}}_+$. The equilibrium solution $r(k) \equiv r_e$ of (1) is *semistable* if it is Lyapunov stable and there exists $\delta > 0$ such that if $r_0 \in \mathcal{B}_\delta(r_e) \cap \overline{\mathbb{R}}_+^q$, then $\lim_{k \rightarrow \infty} r(k)$ exists and converges to a Lyapunov stable equilibrium point. The equilibrium solution $r(k) \equiv r_e$ of (1) is *asymptotically stable* if it is Lyapunov stable and there exists $\delta > 0$ such that if $r_0 \in \mathcal{B}_\delta(r_e) \cap \overline{\mathbb{R}}_+^q$, then $\lim_{k \rightarrow \infty} r(k) = r_e$. Finally, the equilibrium solution $r(k) \equiv r_e$ of (1) is *globally asymptotically stable* if the previous statement holds for all $r_0 \in \overline{\mathbb{R}}_+^q$.

III. THERMODYNAMIC MODELING FOR DISCRETE-TIME DYNAMICAL SYSTEMS

The fundamental and unifying concept in the analysis of complex (large-scale) dynamical systems is the concept of energy. The energy of a state of a dynamical system is the measure of its ability to produce changes (motion) in its own system state as well as changes in the system states of its surroundings. These changes occur as a direct consequence of the energy flow between different subsystems within the dynamical system. Since heat (energy) is a fundamental concept of thermodynamics involving the capacity of hot bodies (more energetic subsystems) to produce work, thermodynamics is a theory of large-scale dynamical systems [1]. As in thermodynamic systems, dynamical systems can exhibit energy (due to friction) that becomes unavailable to do useful work. This in turn contributes to an increase in system entropy; a measure of the tendency of a system to lose the ability to do useful work.

To develop discrete-time compartmental models that are consistent with thermodynamic principles, consider a discrete-time large-scale dynamical system \mathcal{G} involving q interconnected subsystems. Let $E_i : \overline{\mathbb{Z}}_+ \rightarrow \overline{\mathbb{R}}_+$ denote the energy (and hence a nonnegative quantity) of the i th subsystem, let $S_i : \overline{\mathbb{Z}}_+ \rightarrow \mathbb{R}$ denote the external energy supplied to (or extracted from) the i th subsystem, let $\sigma_{ij} : \overline{\mathbb{R}}_+^q \rightarrow \overline{\mathbb{R}}_+$, $i \neq j$, $i, j = 1, \dots, q$, denote the exchange of energy from the j th subsystem to the i th subsystem, and let $\sigma_{ii} : \overline{\mathbb{R}}_+^q \rightarrow \overline{\mathbb{R}}_+$, $i = 1, \dots, q$, denote the energy loss from the i th subsystem. An *energy balance* equation for the i th subsystem yields

$$\Delta E_i(k) = \sum_{j=1, j \neq i}^q [\sigma_{ij}(E(k)) - \sigma_{ji}(E(k))] - \sigma_{ii}(E(k)) + S_i(k), \quad k \geq k_0, \quad (2)$$

or, equivalently, in vector form,

$$E(k+1) = w(E(k)) - d(E(k)) + S(k), \quad k \geq k_0, \quad (3)$$

where $E(k) = [E_1(k), \dots, E_q(k)]^T$, $S(k) = [S_1(k), \dots, S_q(k)]^T$, $d(E(k)) = [\sigma_{11}(E(k)), \dots, \sigma_{qq}(E(k))]^T$, $k \geq k_0$, and $w = [w_1, \dots, w_q]^T : \overline{\mathbb{R}}_+^q \rightarrow \mathbb{R}^q$ is such that

$$w_i(E) = E_i + \sum_{j=1, j \neq i}^q [\sigma_{ij}(E) - \sigma_{ji}(E)], \quad E \in \overline{\mathbb{R}}_+^q. \quad (4)$$

Equation (2) yields a conservation of energy equation and implies that the change of energy stored in the i th subsystem is equal to the external energy supplied to (or extracted from) the i th subsystem plus the energy gained by the i th subsystem from all other subsystems due to subsystem coupling minus the energy dissipated from the i th subsystem. Note that (3) or, equivalently, (2) is a statement reminiscent of the *first law of thermodynamics* for each of the subsystems, with $E_i(\cdot)$, $S_i(\cdot)$, $\sigma_{ij}(\cdot)$, $i \neq j$, and $\sigma_{ii}(\cdot)$, $i = 1, \dots, q$, playing the role of the i th subsystem internal energy, energy supplied to (or extracted from) the i th subsystem, the energy exchange between subsystems due to coupling, and the energy dissipated to the environment, respectively.

To further elucidate that (3) is essentially the statement of the principle of the conservation of energy let the total energy in the discrete-time large-scale dynamical system \mathcal{G} be given by $U \triangleq \mathbf{e}^T E$, $E \in \overline{\mathbb{R}}_+^q$, where $\mathbf{e}^T \triangleq [1, \dots, 1]$, and let the energy received by the discrete-time large-scale dynamical system \mathcal{G} (in forms other than work) over the discrete-time interval $\{k_1, \dots, k_2\}$ be given by $Q \triangleq \sum_{k=k_1}^{k_2} \mathbf{e}^T [S(k) - d(E(k))]$, where $E(k)$, $k \geq k_0$, is the solution to (3). Then, premultiplying (3) by \mathbf{e}^T and using the fact that $\mathbf{e}^T w(E) \equiv \mathbf{e}^T E$, it follows that

$$\Delta U = Q, \quad (5)$$

where $\Delta U \triangleq U(k_2) - U(k_1)$ denotes the variation in the total energy of the discrete-time large-scale dynamical system \mathcal{G} over the discrete-time interval $\{k_1, \dots, k_2\}$. This is a statement of the first law of thermodynamics for the discrete-time large-scale dynamical system \mathcal{G} and gives a precise formulation of the equivalence between variation in system internal energy and heat.

It is important to note that our discrete-time large-scale dynamical system model does not consider work done by the system on the environment nor work done by the environment on the system. Hence, Q can be interpreted physically as the amount of energy that is received by the system in forms other than work. The extension of addressing work performed by and on the system can be easily handled by including an additional state equation, coupled to the energy balance equation (3), involving volume states for each subsystem [1]. Since this slight extension does not alter any of the results of the paper, it is not considered here for simplicity of exposition.

For our large-scale dynamical system model \mathcal{G} , we assume that $\sigma_{ij}(E) = 0$, $E \in \overline{\mathbb{R}}_+^q$, whenever $E_j = 0$, $i, j = 1, \dots, q$. This constraint implies that if the energy of the j th subsystem of \mathcal{G} is zero, then this subsystem cannot supply any energy to its surroundings nor dissipate energy to the environment. Furthermore, for the remainder of this paper we assume that $E_i \geq \sigma_{ii}(E) - S_i - \sum_{j=1, j \neq i}^q [\sigma_{ij}(E) - \sigma_{ji}(E)] = -\Delta E_i$, $E \in \overline{\mathbb{R}}_+^q$, $S \in \mathbb{R}^q$, $i = 1, \dots, q$. This constraint implies that the energy that can be dissipated, extracted, or exchanged by the i th subsystem cannot exceed the current energy in the subsystem. Note that this assumption implies that $E(k) \geq 0$ for all $k \geq k_0$.

Next, premultiplying (3) by \mathbf{e}^T and using the fact that $\mathbf{e}^T w(E) \equiv \mathbf{e}^T E$, it follows that

$$\begin{aligned} \mathbf{e}^T E(k_1) &= \mathbf{e}^T E(k_0) + \sum_{k=k_0}^{k_1-1} \mathbf{e}^T S(k) \\ &\quad - \sum_{k=k_0}^{k_1-1} \mathbf{e}^T d(E(k)), \quad k_1 \geq k_0. \end{aligned} \quad (6)$$

Now, for the discrete-time large-scale dynamical system \mathcal{G} define the input $u(k) \triangleq S(k)$ and the output $y(k) \triangleq d(E(k))$. Hence, it follows from (6) that the discrete-time large-scale dynamical system \mathcal{G} is *lossless* [7] with respect to the *energy supply rate* $r(u, y) = \mathbf{e}^T u - \mathbf{e}^T y$ and with the *energy storage function* $U(E) \triangleq \mathbf{e}^T E$, $E \in \overline{\mathbb{R}}_+^q$. This implies that (see [7] for details)

$$0 \leq U_a(E_0) = U(E_0) = U_r(E_0) < \infty, \quad E_0 \in \overline{\mathbb{R}}_+^q, \quad (7)$$

where

$$U_a(E_0) \triangleq - \inf_{u(\cdot), K \geq k_0} \sum_{k=k_0}^{K-1} (\mathbf{e}^T u(k) - \mathbf{e}^T y(k)), \quad (8)$$

$$U_r(E_0) \triangleq \inf_{u(\cdot), K \geq -k_0+1} \sum_{k=-K}^{k_0-1} (\mathbf{e}^T u(k) - \mathbf{e}^T y(k)), \quad (9)$$

and $E_0 = E(k_0) \in \overline{\mathbb{R}}_+^q$. Since $U_a(E_0)$ is the maximum amount of stored energy which can be extracted from the discrete-time large-scale dynamical system \mathcal{G} at any discrete-time instant K , and $U_r(E_0)$ is the minimum amount of energy which can be delivered to the discrete-time large-scale dynamical system \mathcal{G} to transfer it from a state of minimum potential $E(-K) = 0$ to a given state $E(k_0) = E_0$, it follows from (7) that the discrete-time large-scale dynamical system \mathcal{G} can deliver to its surroundings all of its stored subsystem energies and can store all of the work done to all of its subsystems. In the case where $S(k) \equiv 0$, it follows from (6) and the fact that $\sigma_{ii}(E) \geq 0$, $E \in \overline{\mathbb{R}}_+^q$, $i = 1, \dots, q$, that the zero solution $E(k) \equiv 0$ of the discrete-time large-scale dynamical system \mathcal{G} with the energy balance equation (3) is Lyapunov stable with Lyapunov function $U(E)$ corresponding to the total energy in the system.

The next result shows that the large-scale dynamical system \mathcal{G} is locally controllable.

Proposition 3.1: Consider the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3). Then for every equilibrium state $E_e \in \overline{\mathbb{R}}_+^q$ and every $\varepsilon > 0$ and $T \in \mathbb{Z}_+$, there exist $S_e \in \mathbb{R}^q$, $\alpha > 0$, and $\hat{T} \in \{0, \dots, T\}$ such that for every $\hat{E} \in \overline{\mathbb{R}}_+^q$ with $\|\hat{E} - E_e\| \leq \alpha T$, there exists $S : \{0, \dots, \hat{T}\} \rightarrow \mathbb{R}^q$ such that $\|S(k) - S_e\| \leq \varepsilon$, $k \in \{0, \dots, \hat{T}\}$, and $E(k) = E_e + \frac{(\hat{E} - E_e)}{\hat{T}} k$, $k \in \{0, \dots, \hat{T}\}$.

It follows from Proposition 3.1 that the discrete-time large-scale dynamical system \mathcal{G} with the energy balance equation (3) is *reachable* from and *controllable* to the origin in $\overline{\mathbb{R}}_+^q$. Recall that the discrete-time large-scale dynamical system \mathcal{G} with the energy balance equation (3) is reachable from the origin in $\overline{\mathbb{R}}_+^q$ if, for all $E_0 = E(k_0) \in \overline{\mathbb{R}}_+^q$, there exists a finite time $k_i \leq k_0$ and an input $S(k)$ defined on $\{k_i, \dots, k_0\}$ such that the state $E(k)$, $k \geq k_i$, can be driven from $E(k_i) = 0$ to $E(k_0) = E_0$. Alternatively, \mathcal{G} is

controllable to the origin in $\overline{\mathbb{R}}_+^q$ if, for all $E_0 = E(k_0) \in \overline{\mathbb{R}}_+^q$, there exists a finite time $k_f \geq k_0$ and an input $S(k)$ defined on $\{k_0, \dots, k_f\}$ such that the state $E(k)$, $k \geq k_0$, can be driven from $E(k_0) = E_0$ to $E(k_f) = 0$. We let \mathcal{U}_r denote the set of all admissible bounded energy inputs to the discrete-time large-scale dynamical system \mathcal{G} such that for any $K \geq -k_0$, the system energy state can be driven from $E(-K) = 0$ to $E(k_0) = E_0 \in \overline{\mathbb{R}}_+^q$ by $S(\cdot) \in \mathcal{U}_r$, and we let \mathcal{U}_c denote the set of all admissible bounded energy inputs to the discrete-time large-scale dynamical system \mathcal{G} such that for any $K \geq k_0$, the system energy state can be driven from $E(k_0) = E_0 \in \overline{\mathbb{R}}_+^q$ to $E(K) = 0$ by $S(\cdot) \in \mathcal{U}_c$. Furthermore, let \mathcal{U} be an input space that is a subset of bounded continuous \mathbb{R}^q -valued functions on \mathbb{Z} . The spaces \mathcal{U}_r , \mathcal{U}_c , and \mathcal{U} are assumed to be closed under the shift operator, that is, if $S(\cdot) \in \mathcal{U}$ (respectively, \mathcal{U}_c or \mathcal{U}_r), then the function S_K defined by $S_K(k) = S(k+K)$ is contained in \mathcal{U} (respectively, \mathcal{U}_c or \mathcal{U}_r) for all $K \geq 0$.

The nonlinear energy balance equation (3) can exhibit a full range of nonlinear behavior including bifurcations, limit cycles, and even chaos. However, a thermodynamically consistent energy flow model should ensure that the evolution of the system energy is diffusive (parabolic) in character with convergent subsystem energies. Hence, to ensure a thermodynamically consistent energy flow model we require the following axioms. For the statement of these axioms we first recall the following graph theoretic notions.

Definition 3.1 ([1]): A directed graph $G(\mathcal{C})$ associated with the connectivity matrix $\mathcal{C} \in \mathbb{R}^{q \times q}$ has vertices $\{1, 2, \dots, q\}$ and an arc from vertex i to vertex j , $i \neq j$, if and only if $\mathcal{C}_{(j,i)} \neq 0$. A graph $G(\mathcal{C})$ associated with the connectivity matrix $\mathcal{C} \in \mathbb{R}^{q \times q}$ is a directed graph for which the arc set is symmetric; that is, $\mathcal{C} = \mathcal{C}^T$. We say that $G(\mathcal{C})$ is *strongly connected* if for any ordered pair of vertices (i, j) , $i \neq j$, there exists a *path* (i.e., sequence of arcs) leading from i to j .

Recall that $\mathcal{C} \in \mathbb{R}^{q \times q}$ is *irreducible*, that is, there does not exist a permutation matrix such that \mathcal{C} is cogredient to a lower-block triangular matrix, if and only if $G(\mathcal{C})$ is strongly connected (see Theorem 2.7 of [8]). Let $\phi_{ij}(E) \triangleq \sigma_{ij}(E) - \sigma_{ji}(E)$, $E \in \overline{\mathbb{R}}_+^q$, denote the net energy exchange between subsystems \mathcal{G}_i and \mathcal{G}_j of the discrete-time large-scale dynamical system \mathcal{G} .

Axiom i): For the connectivity matrix $\mathcal{C} \in \mathbb{R}^{q \times q}$ associated with the large-scale dynamical system \mathcal{G} defined by

$$\mathcal{C}_{(i,j)} = \begin{cases} 0, & \text{if } \phi_{ij}(E) \equiv 0, \\ 1, & \text{otherwise,} \\ & i \neq j, \quad i, j = 1, \dots, q, \end{cases} \quad (10)$$

and

$$\mathcal{C}_{(i,i)} = - \sum_{k=1, k \neq i}^q \mathcal{C}_{(k,i)}, \quad i = j, \quad i = 1, \dots, q, \quad (11)$$

rank $\mathcal{C} = q - 1$, and for $\mathcal{C}_{(i,j)} = 1$, $i \neq j$, $\phi_{ij}(E) = 0$ if and only if $E_i = E_j$.

Axiom ii): For $i, j = 1, \dots, q$, $(E_i - E_j)\phi_{ij}(E) \leq 0$, $E \in \overline{\mathbb{R}}_+^q$.

Axiom iii): For $i, j = 1, \dots, q$, $\frac{\Delta E_i - \Delta E_j}{E_i - E_j} \geq -1$, $E_i \neq E_j$.

The fact that $\phi_{ij}(E) = 0$ if and only if $E_i = E_j$, $i \neq j$, implies that subsystems \mathcal{G}_i and \mathcal{G}_j of \mathcal{G} are *connected*;

alternatively, $\phi_{ij}(E) \equiv 0$ implies that \mathcal{G}_i and \mathcal{G}_j are *disconnected*. Axiom *i*) implies that if the energies in the connected subsystems \mathcal{G}_i and \mathcal{G}_j are equal, then energy exchange between these subsystems is not possible. This is a statement consistent with the *zeroth law of thermodynamics* which postulates that temperature equality is a necessary and sufficient condition for thermal equilibrium. Furthermore, it follows from the fact that $\mathcal{C} = \mathcal{C}^T$ and $\text{rank } \mathcal{C} = q - 1$ that the connectivity matrix \mathcal{C} is irreducible which implies that for any pair of subsystems \mathcal{G}_i and \mathcal{G}_j , $i \neq j$, of \mathcal{G} there exists a sequence of connected subsystems of \mathcal{G} that connect \mathcal{G}_i and \mathcal{G}_j . Axiom *ii*) implies that energy is exchanged from more energetic subsystems to less energetic subsystems and is consistent with the *second law of thermodynamics* which states that heat (energy) must flow in the direction of lower temperatures. Furthermore, note that $\phi_{ij}(E) = -\phi_{ji}(E)$, $E \in \overline{\mathbb{R}}_+^q$, $i \neq j$, $i, j = 1, \dots, q$, which implies conservation of energy between lossless subsystems. With $S(k) \equiv 0$, Axioms *i*) and *ii*) along with the fact that $\phi_{ij}(E) = -\phi_{ji}(E)$, $E \in \overline{\mathbb{R}}_+^q$, $i \neq j$, $i, j = 1, \dots, q$, imply that at a given instant of time energy can only be transported, stored, or dissipated but not created and the maximum amount of energy that can be transported and/or dissipated from a subsystem cannot exceed the energy in the subsystem. Finally, Axiom *iii*) implies that for any pair of connected subsystems \mathcal{G}_i and \mathcal{G}_j , $i \neq j$, the energy difference between consecutive time instants is monotonic, that is, $[E_i(k+1) - E_j(k+1)][E_i(k) - E_j(k)] \geq 0$ for all $E_i \neq E_j$, $k \geq k_0$, $i, j = 1, \dots, q$.

Next, we establish a Clausius-type inequality for our thermodynamically consistent energy flow model.

Proposition 3.2: Consider the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3) and assume that Axioms *i*), *ii*), and *iii*) hold. Then for all $E_0 \in \overline{\mathbb{R}}_+^q$, $k_f \geq k_0$, and $S(\cdot) \in \mathcal{U}$ such that $E(k_f) = E(k_0) = E_0$,

$$\begin{aligned} & \sum_{k=k_0}^{k_f-1} \sum_{i=1}^q \frac{S_i(k) - \sigma_{ii}(E(k))}{c + E_i(k+1)} \\ &= \sum_{k=k_0}^{k_f-1} \sum_{i=1}^q \frac{Q_i(k)}{c + E_i(k+1)} \leq 0, \end{aligned} \quad (12)$$

where $c > 0$, $Q_i(k) \triangleq S_i(k) - \sigma_{ii}(E(k))$, $i = 1, \dots, q$, is the amount of net energy (heat) received by the i th subsystem at the k th instant, and $E(k)$, $k \geq k_0$, is the solution to (3) with initial condition $E(k_0) = E_0$. Furthermore, equality holds in (12) if and only if $\Delta E_i(k) = 0$, $i = 1, \dots, q$, and $E_i(k) = E_j(k)$, $i, j = 1, \dots, q$, $i \neq j$, $k \in \{k_0, \dots, k_f - 1\}$.

Inequality (12) is analogous to Clausius' equality and inequality for reversible and irreversible thermodynamics as applied to discrete-time large-scale dynamical systems. It follows from Axiom *i*) and (3) that for the *isolated* discrete-time large-scale dynamical system \mathcal{G} ; that is, $S(k) \equiv 0$ and $d(E(k)) \equiv 0$, the energy states given by $E_e = \alpha e$, $\alpha \geq 0$, correspond to the equilibrium energy states of \mathcal{G} . Thus, we can define an *equilibrium process* as a process where the trajectory of the discrete-time large-scale dynamical system \mathcal{G} stays at the equilibrium point of the isolated system \mathcal{G} . The input that can generate such a trajectory can be given by $S(k) = d(E(k))$, $k \geq k_0$. Alternatively, a *nonequilibrium process* is a process that is not an equilibrium one. Hence, it follows from Axiom *i*) that for an equilibrium process $\phi_{ij}(E(k)) \equiv 0$, $k \geq k_0$, $i \neq j$, $i, j = 1, \dots, q$, and thus, by Proposition 3.2 and $\Delta E_i = 0$, $i = 1, \dots, q$,

inequality (12) is satisfied as an equality. Alternatively, for a nonequilibrium process it follows from Axioms *i*) – *iii*) that (12) is satisfied as a strict inequality.

Next, we give a deterministic definition of entropy for the discrete-time large-scale dynamical system \mathcal{G} that is consistent with the classical thermodynamic definition of entropy.

Definition 3.2: For the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3), a function $\mathcal{S} : \overline{\mathbb{R}}_+^q \rightarrow \mathbb{R}$ satisfying

$$\begin{aligned} \mathcal{S}(E(k_2)) &\geq \mathcal{S}(E(k_1)) \\ &+ \sum_{k=k_1}^{k_2-1} \sum_{i=1}^q \frac{S_i(k) - \sigma_{ii}(E(k))}{c + E_i(k+1)}, \end{aligned} \quad (13)$$

for any $k_2 \geq k_1 \geq k_0$ and $S(\cdot) \in \mathcal{U}$, is called the *entropy* of \mathcal{G} .

Next, we show that (12) guarantees the existence of an entropy function for \mathcal{G} . For this result define the *available entropy* of the large-scale dynamical system \mathcal{G} by

$$\begin{aligned} \mathcal{S}_a(E_0) &\triangleq - \sup_{S(\cdot) \in \mathcal{U}_c, K \geq k_0} \sum_{k=k_0}^{K-1} \sum_{i=1}^q \frac{S_i(k) - \sigma_{ii}(E(k))}{c + E_i(k+1)}, \end{aligned} \quad (14)$$

where $E(k_0) = E_0 \in \overline{\mathbb{R}}_+^q$ and $E(K) = 0$, and define the *required entropy supply* of the large-scale dynamical system \mathcal{G} by

$$\begin{aligned} \mathcal{S}_r(E_0) &\triangleq \sup_{S(\cdot) \in \mathcal{U}_r, K \geq -k_0+1} \sum_{k=-K}^{k_0-1} \sum_{i=1}^q \frac{S_i(k) - \sigma_{ii}(E(k))}{c + E_i(k+1)}, \end{aligned} \quad (15)$$

where $E(-K) = 0$ and $E(k_0) = E_0 \in \overline{\mathbb{R}}_+^q$. Note that the available entropy $\mathcal{S}_a(E_0)$ is the minimum amount of scaled heat (entropy) that can be extracted from the large-scale dynamical system \mathcal{G} in order to transfer it from an initial state $E(k_0) = E_0$ to $E(K) = 0$. Alternatively, the required entropy supply $\mathcal{S}_r(E_0)$ is the maximum amount of scaled heat (entropy) that can be delivered to \mathcal{G} to transfer it from the origin to a given initial state $E(k_0) = E_0$.

Theorem 3.1: Consider the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3) and assume that Axioms *ii*) and *iii*) hold. Then there exists an entropy function for \mathcal{G} . Moreover, $\mathcal{S}_a(E)$, $E \in \overline{\mathbb{R}}_+^q$, and $\mathcal{S}_r(E)$, $E \in \overline{\mathbb{R}}_+^q$, are possible entropy functions for \mathcal{G} with $\mathcal{S}_a(0) = \mathcal{S}_r(0) = 0$. Finally, all entropy functions $\mathcal{S}(E)$, $E \in \overline{\mathbb{R}}_+^q$, for \mathcal{G} satisfy

$$\mathcal{S}_r(E) \leq \mathcal{S}(E) - \mathcal{S}(0) \leq \mathcal{S}_a(E), \quad E \in \overline{\mathbb{R}}_+^q. \quad (16)$$

Remark 3.1: It is important to note that inequality (12) is equivalent to the existence of an entropy function for \mathcal{G} . Sufficiency is simply a statement of Theorem 3.1 while necessity follows from (13) with $E(k_2) = E(k_1)$. For nonequilibrium process with energy balance equation (3), Definition 3.2 does not provide enough information to define the entropy uniquely. This difficulty has long been pointed out in [9] for thermodynamic systems. A similar remark holds for the definition of entropy introduced below.

The next proposition gives a closed-form expression for the entropy of \mathcal{G} .

Proposition 3.3: Consider the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3) and assume that Axioms *ii*) and *iii*) hold. Then the function $\mathcal{S} : \overline{\mathbb{R}}_+^q \rightarrow \mathbb{R}$ given by

$$\mathcal{S}(E) = \mathbf{e}^T \mathbf{log}_e(\mathbf{c}e + E) - q \log_e c, \quad E \in \overline{\mathbb{R}}_+^q, \quad (17)$$

where $\mathbf{log}_e(\mathbf{c}e + E)$ denotes the vector natural logarithm given by $[\log_e(c + E_1), \dots, \log_e(c + E_q)]^T$ and $c > 0$, is an entropy function of \mathcal{G} .

Remark 3.2: Note that the entropy function given by (17) satisfies (13) as an equality for an equilibrium process and as a strict inequality for a nonequilibrium process.

The entropy expression given by (17) is identical in form to the Boltzmann entropy for statistical thermodynamics. Due to the fact that the entropy is indeterminate to the extent of an additive constant, we can place the constant $q \log_e c$ to zero by taking $c = 1$. Since $\mathcal{S}(E)$ given by (17) achieves a maximum when all the subsystem energies E_i , $i = 1, \dots, q$, are equal, entropy can be thought of as a measure of the tendency of a system to lose the ability to do useful work, lose order, and settle to a more homogenous state.

Next, we introduce a *new* and dual notion to entropy, namely, ectropy, describing the status quo of the discrete-time large-scale dynamical system \mathcal{G} . First, however, we present a dual inequality to inequality (12) that holds for our thermodynamically consistent energy flow model.

Proposition 3.4: Consider the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3) and assume that Axioms *i*), *ii*), and *iii*) hold. Then for all $E_0 \in \overline{\mathbb{R}}_+^q$, $k_f \geq k_0$, and $S(\cdot) \in \mathcal{U}$ such that $E(k_f) = E(k_0) = E_0$,

$$\begin{aligned} & \sum_{k=k_0}^{k_f-1} \sum_{i=1}^q E_i(k+1)[S_i(k) - \sigma_{ii}(E(k))] \\ &= \sum_{k=k_0}^{k_f-1} \sum_{i=1}^q E_i(k+1)Q_i(k) \geq 0, \end{aligned} \quad (18)$$

where $E(k)$, $k \geq k_0$, is the solution to (3) with initial condition $E(k_0) = E_0$. Furthermore, equality holds in (18) if and only if $\Delta E_i = 0$ and $E_i = E_j$, $i, j = 1, \dots, q$, $i \neq j$.

Note that inequality (18) is satisfied as an equality for an equilibrium process and as a strict inequality for a nonequilibrium process. Next, we present the definition of ectropy for the discrete-time large-scale dynamical system \mathcal{G} .

Definition 3.3: For the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3), a function $\mathcal{E} : \overline{\mathbb{R}}_+^q \rightarrow \mathbb{R}$ satisfying

$$\begin{aligned} \mathcal{E}(E(k_2)) &\leq \mathcal{E}(E(k_1)) \\ &+ \sum_{k=k_1}^{k_2-1} \sum_{i=1}^q E_i(k+1)[S_i(k) - \sigma_{ii}(E(k))], \end{aligned} \quad (19)$$

for any $k_2 \geq k_1 \geq k_0$ and $S(\cdot) \in \mathcal{U}$, is called the *ectropy* of \mathcal{G} .

For the next result define the *available ectropy* of the

large-scale dynamical system \mathcal{G} by

$$\begin{aligned} \mathcal{E}_a(E_0) &\triangleq - \inf_{S(\cdot) \in \mathcal{U}_c, K \geq k_0} \sum_{k=k_0}^{K-1} \sum_{i=1}^q E_i(k+1)[S_i(k) - \sigma_{ii}(E(k))], \end{aligned} \quad (20)$$

where $E(k_0) = E_0 \in \overline{\mathbb{R}}_+^q$ and $E(K) = 0$, and the *required ectropy supply* of the large-scale dynamical system \mathcal{G} by

$$\begin{aligned} \mathcal{E}_r(E_0) &\triangleq \inf_{S(\cdot) \in \mathcal{U}_r, K \geq -k_0+1} \sum_{k=-K}^{k_0-1} \sum_{i=1}^q E_i(k+1)[S_i(k) \\ &- \sigma_{ii}(E(k))], \end{aligned} \quad (21)$$

where $E(-K) = 0$ and $E(k_0) = E_0 \in \overline{\mathbb{R}}_+^q$. Note that the available ectropy $\mathcal{E}_a(E_0)$ is the maximum amount of scaled heat (ectropy) that can be extracted from the large-scale dynamical system \mathcal{G} in order to transfer it from an initial state $E(k_0) = E_0$ to $E(K) = 0$. Alternatively, the required ectropy supply $\mathcal{E}_r(E_0)$ is the minimum amount of scaled heat (ectropy) that can be delivered to \mathcal{G} to transfer it from an initial state $E(-K) = 0$ to a given state $E(k_0) = E_0$.

Theorem 3.2: Consider the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3) and assume that Axioms *ii*) and *iii*) hold. Then there exists an ectropy function for \mathcal{G} . Moreover, $\mathcal{E}_a(E)$, $E \in \overline{\mathbb{R}}_+^q$, and $\mathcal{E}_r(E)$, $E \in \overline{\mathbb{R}}_+^q$, are possible ectropy functions for \mathcal{G} with $\mathcal{E}_a(0) = \mathcal{E}_r(0) = 0$. Finally, all ectropy functions $\mathcal{E}(E)$, $E \in \overline{\mathbb{R}}_+^q$, for \mathcal{G} satisfy

$$\mathcal{E}_a(E) \leq \mathcal{E}(E) - \mathcal{E}(0) \leq \mathcal{E}_r(E), \quad E \in \overline{\mathbb{R}}_+^q. \quad (22)$$

The next proposition gives a closed-form expression for the ectropy of \mathcal{G} .

Proposition 3.5: Consider the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3) and assume that Axioms *ii*) and *iii*) hold. Then the function $\mathcal{E} : \overline{\mathbb{R}}_+^q \rightarrow \mathbb{R}$ given by

$$\mathcal{E}(E) = \frac{1}{2} E^T E, \quad E \in \overline{\mathbb{R}}_+^q, \quad (23)$$

is an ectropy function of \mathcal{G} .

Remark 3.3: Note that the ectropy function given by (23) satisfies (19) as an equality for an equilibrium process and as a strict inequality for a nonequilibrium process.

It follows from (23) that ectropy is a measure of the extent to which the system energy deviates from a homogeneous state. Thus, ectropy is the dual of entropy and is a measure of the tendency of the discrete-time large-scale dynamical system \mathcal{G} to do useful work and grow more organized.

Inequality (13) is analogous to Clausius' inequality for equilibrium and nonequilibrium thermodynamics as applied to discrete-time large-scale dynamical systems, while inequality (19) is an anti-Clausius' inequality. Moreover, for the ectropy function defined by (23), a thermodynamically consistent discrete-time large-scale dynamical system is *dissipative* [7] with respect to the supply rate $E^T S$ and with storage function corresponding to the system ectropy $\mathcal{E}(E)$. For the entropy function given by (17) note that $\mathcal{S}(0) = 0$, or, equivalently, $\lim_{E \rightarrow 0} \mathcal{S}(E) = 0$, which is consistent with the *third law of thermodynamics* (Nernst's theorem) which states that the entropy of every system at absolute zero can always be taken to be equal to zero.

For the isolated discrete-time large-scale dynamical system \mathcal{G} , (13) yields the fundamental inequality

$$\mathcal{S}(E(k_2)) \geq \mathcal{S}(E(k_1)), \quad k_2 \geq k_1. \quad (24)$$

Inequality (24) implies that, for any dynamical change in an isolated (i.e., $S(k) \equiv 0$ and $d(E(k)) \equiv 0$) discrete-time large-scale system, the entropy of the final state can never be less than the entropy of the initial state. It is important to stress that this result holds for an isolated dynamical system. It is however possible with energy supplied from an external dynamical system (e.g., a controller) to reduce the entropy of the discrete-time large-scale dynamical system. The entropy of both systems taken together however cannot decrease. The above observations imply that when an isolated discrete-time large-scale dynamical system with thermodynamically consistent energy flow characteristics (i.e., Axioms *i*)–*iii*) hold) is at a state of maximum entropy consistent with its energy, it cannot be subject to any further dynamical change since any such change would result in a decrease of entropy. This of course implies that the state of *maximum entropy* is the stable state of an isolated system and this state has to be semistable.

Analogously, it follows from (19) that for an isolated discrete-time large-scale dynamical system \mathcal{G} the fundamental inequality

$$\mathcal{E}(E(k_2)) \leq \mathcal{E}(E(k_1)), \quad k_2 \geq k_1, \quad (25)$$

is satisfied, which implies that the ectropy of the final state of \mathcal{G} is always less than or equal to the ectropy of the initial state of \mathcal{G} . Hence, for the isolated large-scale dynamical system \mathcal{G} the entropy increases if and only if the ectropy decreases. Thus, the state of *minimum ectropy* is the stable state of an isolated system and this equilibrium state has to be semistable. The next theorem concretizes the above observations.

Theorem 3.3: Consider the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3) with $S(k) \equiv 0$ and $d(E) \equiv 0$, and assume that Axioms *i*)–*iii*) hold. Then for every $\alpha \geq 0$, $\alpha \mathbf{e}$ is a Lyapunov equilibrium state of (3). Furthermore, $E(k) \rightarrow \frac{1}{q} \mathbf{e} \mathbf{e}^T E(k_0)$ as $k \rightarrow \infty$ and $\frac{1}{q} \mathbf{e} \mathbf{e}^T E(k_0)$ is a semistable equilibrium state. Finally, if for some $m \in \{1, \dots, q\}$, $\sigma_{mm}(E) \geq 0$, $E \in \mathbb{R}_+^q$, and $\sigma_{mm}(E) = 0$ if and only if $E_m = 0^1$, then the zero solution $E(k) \equiv 0$ to (3) is a globally asymptotically stable equilibrium state of (3).

Theorem 3.3 implies that the steady-state value of the energy in each subsystem \mathcal{G}_i of the isolated large-scale dynamical system \mathcal{G} is equal, that is, the steady-state energy of the isolated discrete-time large-scale dynamical system \mathcal{G} given by $E_\infty = \frac{1}{q} \mathbf{e} \mathbf{e}^T E(k_0) = \left[\frac{1}{q} \sum_{i=1}^q E_i(k_0) \right] \mathbf{e}$ is uniformly distributed over all subsystems of \mathcal{G} . This phenomenon is known as *equipartition of energy* [1] and is an emergent behavior in thermodynamic systems. The next proposition shows that among all possible energy distributions in the discrete-time large-scale dynamical system \mathcal{G} , energy equipartition corresponds to the minimum value of the system's ectropy and the maximum value of the system's entropy.

Proposition 3.6: Consider the discrete-time large-scale dynamical system \mathcal{G} with energy balance equation (3), let

¹The assumption $\sigma_{mm}(E) \geq 0$, $E \in \mathbb{R}_+^q$, and $\sigma_{mm}(E) = 0$ if and only if $E_m = 0$ for some $m \in \{1, \dots, q\}$ implies that if the m th subsystem possesses no energy, then this subsystem cannot dissipate energy to the environment. Conversely, if the m th subsystem does not dissipate energy to the environment, then this subsystem has no energy.

$\mathcal{E} : \mathbb{R}_+^q \rightarrow \mathbb{R}$ and $\mathcal{S} : \mathbb{R}_+^q \rightarrow \mathbb{R}$ denote the ectropy and entropy of \mathcal{G} given by (23) and (17), respectively, and define $\mathcal{D}_c \triangleq \{E \in \mathbb{R}_+^q : \mathbf{e}^T E = \beta\}$, where $\beta \geq 0$. Then,

$$\arg \min_{E \in \mathcal{D}_c} (\mathcal{E}(E)) = \arg \max_{E \in \mathcal{D}_c} (\mathcal{S}(E)) = E^* = \frac{\beta}{q} \mathbf{e}. \quad (26)$$

Furthermore, $\mathcal{E}_{\min} \triangleq \mathcal{E}(E^*) = \frac{1}{2} \frac{\beta^2}{q}$ and $\mathcal{S}_{\max} \triangleq \mathcal{S}(E^*) = q \log_e \left(c + \frac{\beta}{q} \right) - q \log_e c$.

It follows from (24), (25), and Proposition 3.6 that conservation of energy necessarily implies nonconservation of ectropy and entropy. Hence, in an isolated discrete-time large-scale dynamical system \mathcal{G} all the energy, though always conserved, will eventually be degraded (diluted) to the point where it cannot produce any useful work. Hence, all motion would cease and the dynamical system would be fated to a state of eternal rest (semistability) wherein all subsystems will possess identical energies (energy equipartition). Ectropy would be a minimum and entropy would be a maximum giving rise to a state of absolute disorder. This is precisely what is known in theoretical physics as the *heat death of the universe* [1].

IV. CONCLUSION

Motivated by energy flow modeling of large-scale interconnected systems, in this paper we develop discrete-time nonlinear compartmental models that are consistent with thermodynamic principles. Specifically, using a discrete-time large-scale systems perspective, we develop some of the key properties of thermodynamic systems involving conservation of energy and nonconservation of entropy and ectropy using dynamical systems theory. The concept of entropy for a large-scale dynamical system is defined and shown to be consistent with the classical thermodynamic definition of entropy.

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