

COMPARTMENTAL MODELING AND SECOND-MOMENT ANALYSIS OF STATE SPACE SYSTEMS*

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Abstract. Compartmental models involve nonnegative state variables that exchange mass, energy, or other quantities in accordance with conservation laws. Such models are widespread in biology and economics. In this paper a connection is made between arbitrary (not necessarily nonnegative) state space systems and compartmental models. Specifically, for an arbitrary state space model with additive white noise, the nonnegative-definite second-moment matrix is characterized by a Lyapunov differential equation. Kronecker and Hadamard (Schur) matrix algebra is then used to derive an equation that characterizes the dynamics of the diagonal elements of the second-moment matrix. Since these diagonal elements are nonnegative, they can be viewed, in certain cases, as the state variables of a compartmental model. This paper examines weak coupling conditions under which the steady-state values of the diagonal elements actually satisfy a steady-state compartmental model.

Key words. stochastic models, power flow, nonnegative matrices

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1. Introduction. Analysis and design methodologies based upon worst-case behavior can be unduly pessimistic for applications in which system behavior includes highly improbable events. It is thus our goal to undertake a probabilistic approach to account for (or, more aptly, to *ignore*) unlikely behavior to achieve higher performance and more realistic predictions. Accordingly, we consider an H_2 /white noise (as opposed to an H_∞/L_2) system and signal model as a starting point. Now, however, we seek system models that ignore detailed *microscopic* modeling data while focussing on the most likely *macroscopic* phenomena. Our paradigm is heat flow in which molecular motion is highly uncertain, whereas energy flows, with virtual certainty, from hot objects to cold objects.

Most probable motion in dynamical systems is the traditional province of statistical mechanics, which normally deals with very large (say, 10^{23}) interacting components. Our challenge in the field of modeling for robust control is to develop a useful theory of “statistical mechanics of moderate-sized systems.” Such a theory does not currently exist due to the emphasis by physicists on large stochastic systems as well as the emphasis by engineers, dynamicists, and control theorists on relatively small deterministic systems. It is our view that a “middle ground theory” is needed to fill the gap between these worlds. The benefits of such a theory include the means to overcome the inherent limitations of worst-case design. The present paper is directed toward this goal.

To begin we shall focus on dynamical systems that involve subsystems or states whose values are nonnegative quantities [1]–[13]. Dynamical models of such systems are based upon the physics of the processes by which various quantities are exchanged by the coupled subsystems. In addition, conservation laws are used to account for the possibly macroscopic transfer (or flow) of such quantities among subsystems. Models for this class of systems are known as *compartmental* models.

The range of application of compartmental models is quite large. Their usage is widespread in biology and ecology [10], [12], while closely related ideas appear in economics [6, Chap. 9]. Our interest in compartmental models arises from electrical and mechanical engineering applications. Thus far there has been little direct connection between these engineering disciplines and compartmental modeling since classical

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(R, L, C) circuit models and (M, D, K) structural models are not cast in terms of inherently nonnegative quantities and do not explicitly invoke conservation laws.

The goal of this paper is to demonstrate a direct connection between arbitrary linear dynamical systems in state space form and compartmental models. The key to this connection is the recognition that even for arbitrary systems that do not explicitly involve nonnegative quantities (such as the (R, L, C) and (M, D, K) models mentioned above), it is possible to identify nonnegative quantities that do behave like compartmental models with conservation laws. In certain specific cases such connections have already been demonstrated, albeit, usually without recognition of compartmental concepts. Examples include energy flow and power transfer in random media [14]–[17], dissipative circuits [18]–[27], mechanical systems [28]–[30], coupled structures [31]–[46], and networks of queues [47] and [48]. A compartmental-like description of coupled structures is given in [35].

In each of the above applications, the key to formulating the system dynamics in compartmental form is to characterize nonnegative quantities that arise from the underlying physical phenomena. The reason that such models have not been more widely used is that physical principles such as Kirchhoff's laws and Newton's law are not usually formulated in terms of subsystem interaction and energy transfer. However, once the underlying laws of physics have been formulated as a dynamical system, it is often possible to reformulate these dynamics in terms of energy transfer. There are at least three mathematical formulations that may give rise to compartmental models:

- (i) root mean square (rms) averaging of system states over time within a deterministic formulation,
- (ii) averaging system states over the statistics of stochastic disturbances, and
- (iii) averaging system states over the statistics of uncertain parameters.

The nonnegative quantities that arise from these formulations are then simply the mean-square averages of the original not-necessarily nonnegative states. In this paper we consider (ii), while approach (iii) underlies much of Statistical Energy Analysis [31]–[42] and has been explored in [49] and [50]. The averaging techniques developed in [51]–[53] are also related to (iii). The results of this paper may also be applicable to large-scale systems problems [54]–[59]. Such connections remain to be explored.

The goal of this paper is to establish some basic mathematical results that demonstrate how compartmental models arise from a second-moment analysis of state space systems. Physical interpretation of the derived compartmental models will not concern us here, while connections to circuit theory and dynamics will be explored elsewhere. Indeed, the above allusions to electrical and mechanical systems should be viewed as purely motivational. Within the paper we shall, however, use “energy” and “power” terminology as generic language to facilitate the discussion.

After introducing some global notation at the end of this section, we proceed in § 2 to summarize some basic properties of compartmental models. Using [6] as our principal reference, we show that compartmental models are confined to a nonnegative state space (Proposition 2.1) and then give necessary and sufficient conditions for the existence of a steady-state equilibrium energy distribution (Proposition 2.2). Sufficient conditions are also given (Corollary 2.2) under which the steady-state distribution is uniform. This phenomenon is known as “equipartition of energy” [34], [41], [50] and is also related to the notion of a “monotemperatonic” system [21]. We stress that although many of these results are well known [3], [6], they are restated here in a concise and unified format that supports the development in later sections.

Specializing to the asymptotically stable case, we then consider the problem of determining the steady-state energy distribution in the limit of strong coupling, that is, the

case in which the off-diagonal terms in the dynamics matrix become arbitrarily large (Proposition 2.4). As a special case of this result we state conditions under which energy equipartition occurs (Corollary 2.3).

In § 3 we shift gears and undertake an analysis of the nonnegative-definite¹ second-moment matrix of an arbitrary (that is, not-necessarily compartmental) n th order asymptotically stable complex-valued system subjected to additive white noise disturbances. Specifically, we rearrange the elements of the $n \times n$ second-moment matrix into an n^2 -dimensional vector whose first n components are the diagonal elements of the second-moment matrix, and whose last $n^2 - n$ components are the off-diagonal elements. Our ability to do this is based upon the following crucial fact: *the diagonal elements of a (complex, Hermitian) nonnegative-definite matrix are (real and) nonnegative.*²

The central result of § 3 is the derivation of an explicit equation that governs the evolution of the diagonal elements of the second-moment equation. As can be seen from (3.18), this equation involves the unusual nonnegative matrix coefficient $e^{Ft} \circ e^{\bar{F}t}$, where F is the dynamics matrix of the original arbitrary (not-necessarily compartmental) state space system, and “ \circ ” denotes Hadamard (Schur) product. Since this system has dynamics that are more complex than an n th order state space system, we confine our attention in § 4 to the steady-state energy distribution.

The goal of § 4 is to determine an n th order state space system whose steady-state solution coincides with the steady-state limit of the nonnegative diagonal system. This requirement leads to a derived dynamics matrix (see (4.12)) involving the elements of the dynamics matrix of the original state space model. To prove that the induced model is asymptotically stable, we consider the case of weak off-diagonal coupling which leads to an M -matrix condition and implies asymptotic stability. A final scaling of the nonnegative system in § 5 shows that in this case the derived model is, in fact, a compartmental model. Finally, notation and identities involving Kronecker and Hadamard products appear in the Appendix.

Notation.

| | |
|---|---|
| \mathbb{E} | expectation |
| \mathbb{R}, \mathbb{C} | real field, complex field |
| $\mathbb{R}^{r \times s}, \mathbb{C}^{r \times s}$ | $r \times s$ real, complex matrices |
| I_r or I | $r \times r$ identity matrix |
| j | $\sqrt{-1}$ |
| A_{kl} | (k, l) -element of $A \in \mathbb{C}^{r \times s}$ (or a subblock of A) |
| $\text{Re } A, \text{Im } A$ | real, imaginary part of $A \in \mathbb{C}^{r \times s}$ |
| \bar{A}, A^T, A^* | conjugate, transpose, complex conjugate transpose |
| $\mathcal{R}(A), \mathcal{N}(A)$ | range and null space of $A \in \mathbb{R}^{r \times s}$ |
| $A \geq \geq 0$ | $A \in \mathbb{R}^{r \times s}$ is a nonnegative matrix |
| $A \circ B$ | Hadamard (Schur) (element-by-element) product |
| \mathbf{e} | $[1 \ 1 \cdots 1]^T$ (boldface distinguishes from exponential) |
| $\text{col}_i(A)$ | i th column of A |
| e_i | i th column of I_r |
| \mathcal{E}_{ij}, I_{ji} | see Appendix |
| $\text{diag}(a_1, \dots, a_n)$ | $n \times n$ matrix with diagonal elements a_1, \dots, a_n |
| $\{A\}, \langle A \rangle$ | diagonal, off-diagonal part of $A \in \mathbb{C}^{r \times r}$ (see Appendix) |
| $\otimes, \oplus, \text{vec}, \text{vecd}, \text{veco}$ | see Appendix |

¹ Throughout the paper a nonnegative-definite matrix is assumed to be Hermitian.

² Since this paper uses both nonnegative matrices and nonnegative-definite matrices in close proximity, care must be taken to note the distinction.

2. Analysis of compartmental models. To begin we consider a system comprised of compartments or subsystems that interact by exchanging some quantity such as mass, energy, fluid, etc. We shall use energy and power analogies for generic terminology. By applying conservation of energy, energy flow among subsystems and the external environment as shown in Fig. 1 leads to the energy balance equation

$$(2.1) \quad \dot{E}_i(t) = -\sigma_{ii}E_i(t) + \sum_{\substack{j=1 \\ j \neq i}}^n \Pi_{ij}(t) + P_i(t), \quad t \geq 0, \quad i = 1, \dots, n,$$

where, for $i = 1, \dots, n$,

- $E_i(t)$ = energy of the i th subsystem,
- σ_{ii} = loss coefficient of the i th subsystem, $\sigma_{ii} \geq 0$,
- $P_i(t)$ = external power applied to the i th subsystem, $P_i(t) \geq 0, t \geq 0$,
- $\Pi_{ij}(t)$ = net energy flow from the j th subsystem to the i th subsystem, $j \neq i$.

As depicted in Fig. 1, it is assumed that $\Pi_{ij}(t)$ is of the form

$$(2.2) \quad \Pi_{ij}(t) = \sigma_{ij}E_j(t) - \sigma_{ji}E_i(t), \quad t \geq 0,$$

where $\sigma_{ij} \geq 0, i \neq j, i, j = 1, \dots, n$. Note that $\Pi_{ji}(t) = -\Pi_{ij}(t), t \geq 0$. Assembling (2.1) and (2.2) into matrix form yields the overall systems model

$$(2.3) \quad \dot{E}(t) = AE(t) + P(t), \quad t \geq 0,$$

where

$$E(t) \triangleq [E_1(t) \cdots E_n(t)]^T, \quad P(t) \triangleq [P_1(t) \cdots P_n(t)]^T,$$

and $A = [A_{ij}]_{i,j=1}^n$ is defined by

$$(2.4) \quad A_{ii} \triangleq -\sum_{j=1}^n \sigma_{ji}, \quad i = 1, \dots, n,$$

$$(2.5) \quad A_{ij} \triangleq \sigma_{ij}, \quad i \neq j, \quad i, j = 1, \dots, n.$$

Letting $\sigma \triangleq [\sigma_{ij}]_{i,j=1}^n$ and using the matrix operators introduced in the Appendix, the matrix A can be written compactly as

$$A = -\text{vecd}^{-1}(\sigma^T \mathbf{e}) + \langle \sigma \rangle.$$

As shown in the Appendix, the operator “vecd” extracts the diagonal elements of a matrix to form a column vector, while “vecd⁻¹” transforms a column vector into a

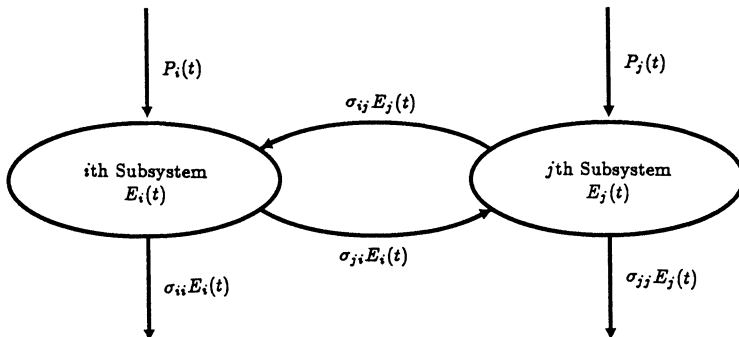


FIG. 1. Compartmental model involving interconnected subsystems.

diagonal matrix. Furthermore, $\langle \sigma \rangle$ denotes the off-diagonal matrix comprised of only the off-diagonal elements of σ with the diagonal elements replaced by zeros.

An important special form of (2.2) arises when $\sigma_{ij} = \sigma_{ji}$ for some $i \neq j$. In this case $\Pi_{ij}(t)$ can be written as

$$(2.6) \quad \Pi_{ij}(t) = \sigma_{ij}[E_j(t) - E_i(t)], \quad t \geq 0,$$

which can be interpreted thermodynamically as saying that heat flow is proportional to temperature difference. Note that A is symmetric if and only if σ is symmetric.

The solution $E(t)$ to (2.3) can be written explicitly as

$$(2.7) \quad E(t) = e^{At}E(0) + \int_0^t e^{A(t-s)}P(s) ds,$$

where the function $P(\cdot)$ is assumed to be such that the integral in (2.7) exists. To analyze (2.7), we begin by noting that A is *essentially nonnegative* [13], that is, the off-diagonal elements of A are nonnegative. Equivalently, $-A$ is a *Z-matrix* [6], that is, $-A$ has nonpositive off-diagonal elements. The following lemma concerns the exponential of an essentially nonnegative matrix. Variations of this result appear in [6, p. 146], [13, p. 74], [55, p. 37], and [60, p. 207].

LEMMA 2.1. *Let $B \in \mathbb{R}^{n \times n}$. Then B is essentially nonnegative if and only if e^{Bt} is nonnegative for all $t \geq 0$.*

Proof. If B is essentially nonnegative, then there exists $\beta > 0$ sufficiently large such that $\hat{B} \triangleq \beta I + B$ is nonnegative. Consequently, $e^{\hat{B}t}$ is nonnegative for all $t \geq 0$, and thus $e^{Bt} = e^{-\beta t}e^{\hat{B}t}$ is nonnegative for all $t \geq 0$. Conversely, suppose that $B_{ij} < 0$ for some $i \neq j$. Then, since $(e^{Bt})_{ij} = tB_{ij} + O(t^2)$ as $t \rightarrow 0$ for $i \neq j$, it follows that $(e^{Bt})_{ij} < 0$ for some $t > 0$ sufficiently small. Hence e^{Bt} is not nonnegative for all $t \geq 0$. \square

Since A is essentially nonnegative, its exponential is nonnegative on $[0, \infty)$. If $E(0)$ and $P(t)$ are both nonnegative, then it follows immediately from (2.7) that $E(t)$ is nonnegative.

PROPOSITION 2.1. *Suppose that $E(0) \geq 0$ and $P(t) \geq 0, t \geq 0$. Then the solution $E(t)$ to (2.3) is nonnegative for all $t \geq 0$.*

Henceforth we focus on the case in which the externally applied power $P(t)$ is constant, that is, $P(t) \equiv P$. In this case (2.3) and (2.7) become

$$(2.8) \quad \dot{E}(t) = AE(t) + P, \quad t \geq 0,$$

and

$$(2.9) \quad E(t) = e^{At}E(0) + \int_0^t e^{As} dsP, \quad t \geq 0.$$

The following lemma summarizes several properties of A that are useful in analyzing (2.9). Recall [61] that the *index* k of a real matrix M , denoted $\text{ind}(M)$, is defined to be the smallest nonnegative integer k such that $\text{rank } M^k = \text{rank } M^{k+1}$. (Here $M^0 \triangleq I$.) Equivalently, $\text{ind}(M)$ is the size of the largest Jordan block of M associated with the eigenvalue zero. Furthermore, recall that if $\text{ind}(M) \leq 1$, then the Drazin inverse M^D specializes to the group inverse $M^\#$ of M . It can be seen that $\text{ind}(M) \leq 1$ and every eigenvalue of M either has negative real part or is zero if and only if $\lim_{t \rightarrow \infty} e^{Mt}$ exists. In this case M is called *semistable*. Finally, let $\mathcal{R}(M)$ and $\mathcal{N}(M)$ denote the range and nullspace of M , respectively.

LEMMA 2.2. *The matrix A defined by (2.4), (2.5) has the following properties:*

- (i) $-A$ is an M -matrix,
- (ii) If λ is an eigenvalue of A then either $\text{Re } \lambda < 0$ or $\lambda = 0$,
- (iii) $\text{ind}(A) \leq 1$,
- (iv) A is semistable, and $\lim_{t \rightarrow \infty} e^{At} = I - AA^\# \geq 0$,
- (v) $\mathcal{R}(A) = \mathcal{N}(I - AA^\#)$, $\mathcal{N}(A) = \mathcal{R}(I - AA^\#)$,
- (vi) $\int_0^t e^{As} ds = A^\#(e^{At} - I) + (I - AA^\#)t$, $t \geq 0$,
- (vii) $\int_0^\infty e^{As} dsP$ exists if and only if $P \in \mathcal{R}(A)$,
- (viii) If $P \in \mathcal{R}(A)$, then $\int_0^\infty e^{As} dsP = -A^\#P$,
- (ix) If $P \in \mathcal{R}(A)$ and $P \geq 0$, then $-A^\#P \geq 0$,
- (x) A is nonsingular if and only if $-A$ is a nonsingular M -matrix,
- (xi) If A is nonsingular, then A is asymptotically stable and $-A^{-1} \geq 0$.

Proof. Since $-A^T e \geq 0$ and $-A$ is a Z -matrix, it follows from [62, Thm. 1, p. 237] or [6, Exercise 6.4.14, p. 155] that $-A^T$, and hence $-A$, is an M -matrix with ‘‘property c ’’ (see [6, Def. 6.4.10, p. 152]), which proves (i). Since $-A$ is an M -matrix, it follows from [6, Prop. (E_{11}), p. 150] that the real part of each nonzero eigenvalue of A is negative, which proves (ii). From [6, Lemma 6.4.11, p. 153], it follows that $\text{ind}(A) \leq 1$, thus proving (iii). To prove (iv), write $A = S \begin{bmatrix} A_0 & 0 \\ 0 & 0 \end{bmatrix} S^{-1}$, where A_0 is asymptotically stable. Then

$$e^{At} = S \begin{bmatrix} e^{A_0 t} & 0 \\ 0 & I \end{bmatrix} S^{-1} \rightarrow S \begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix} S^{-1} = I - AA^\# \quad \text{as } t \rightarrow \infty,$$

which proves (iv). Note that $I - AA^\#$ is nonnegative since e^{At} is nonnegative for all $t \geq 0$. To prove (v), note that if $(I - AA^\#)x = 0$, then $x = AA^\#x \in \mathcal{R}(A)$. Conversely, if $x \in \mathcal{R}(A)$, then there exists $y \in \mathbb{R}^n$ such that $x = Ay$ so that $AA^\#x = AA^\#Ay = Ay = x$. The second identity follows similarly. Next, (vi) follows from [61, Thm. 9.2.4] and can be verified directly. Statement (vii) is a direct consequence of (v) and (vi), while (viii) follows from (iv) and (vi). Next, (ix) follows from (viii) and the fact that $e^{At} \geq 0$, $t \geq 0$. Finally, (x) follows from (i) or [6, p. 137], and (xi) follows from (ii) and (ix) with $P = e_i$, $i = 1, \dots, n$. \square

Remark 2.1. Properties (ii) and (iii) imply that the homogeneous system $\dot{E}(t) = AE(t)$ is stable in the sense of Lyapunov. This result is given by [62, Thm. 1] in terms of the set \mathcal{WL} . The same result is given by [3, Lemmas 1 and 2] and is attributed to [1]. The result (ix) that $x \in \mathcal{R}(A)$ and $x \geq 0$ imply that $-A^\#x \geq 0$ is given by [63, Thm. 3].

By using Lemma 2.2 we can obtain an expression for the steady-state energy distribution $\lim_{t \rightarrow \infty} E(t)$. For notational convenience we denote this limit simply by E .

PROPOSITION 2.2. *Suppose that $E(0) \geq 0$ and $P \geq 0$ and let $E(t)$ be given by (2.9). Then $E \triangleq \lim_{t \rightarrow \infty} E(t)$ exists if and only if $P \in \mathcal{R}(A)$. In this case E is given by*

$$(2.10) \quad E = (I - AA^\#)E(0) - A^\#P,$$

and $E \geq 0$. If, in addition, A is nonsingular, then E exists for all $P \geq 0$ and is given by

$$(2.11) \quad E = -A^{-1}P.$$

In equilibrium, the dynamic system (2.8) becomes

$$(2.12) \quad 0 = AE + P.$$

We now show that the steady-state solution (2.10) is in fact an equilibrium solution to (2.8) and, furthermore, all solutions to (2.12) are of the form (2.10).

PROPOSITION 2.3. *Let $P \in \mathbb{R}^n$. Then (2.12) has a solution $E \in \mathbb{R}^n$ if and only if $P = AA^\#P$. Furthermore, $E \in \mathbb{R}^n$ is a solution to (2.12) if and only if there exists $E(0) \in \mathbb{R}^n$ such that (2.10) is satisfied.*

Proof. Clearly, (2.12) has a solution $E \in \mathbb{R}^n$ if and only if $P \in \mathcal{R}(A)$. By (v) of Lemma 2.2, $P \in \mathcal{R}(A)$ if and only if $P \in \mathcal{N}(I - AA^\#)$, that is, $P = AA^\#P$. Next, it is easy to verify that E given by (2.10) is a solution to (2.12). Conversely, if E satisfies (2.12) then $z \triangleq E + A^\#P$ is in the null space of A . Since by (v) of Lemma 2.2 the null space of A coincides with the range of $I - AA^\#$, it follows that there exists $E(0) \in \mathbb{R}^n$ such that $z = (I - AA^\#)E(0)$, which yields (2.10). \square

Remark 2.2. Proposition 2.3 is entirely analogous to the standard result involving the Moore–Penrose generalized inverse (see, for example, [64, p. 37]). Except for the necessity of the second statement, the result is given by [65, Lemma 5.1].

Writing $E = [E_1 \cdots E_n]^T$ and $P = [P_1 \cdots P_n]^T$, the i th component of (2.12) can be written as

$$(2.13) \quad 0 = -\sigma_{ii}E_i + \sum_{\substack{j=1 \\ j \neq i}}^n [\sigma_{ij}E_j - \sigma_{ji}E_i] + P_i,$$

which can be viewed as an energy balance relation.

When the rank of A is equal to $n - 1$, it is possible to simplify expression (2.10). The following lemma will be useful.

LEMMA 2.3. *Suppose $\text{rank } A = n - 1$ and let $v \in \mathbb{R}^n$ satisfy $Av = 0$. Then either $v \geq 0$ or $-v \geq 0$.*

Proof. Since $v \in \mathcal{N}(A)$, it follows from (v) of Lemma 2.2 that $v \in \mathcal{R}(I - AA^\#)$. Since $\text{rank } A = n - 1$, it follows that $\mathcal{N}(A)$ is one dimensional and thus $\text{rank}(I - AA^\#) = 1$. By (iv) of Lemma 2.2, $I - AA^\#$ is also nonnegative. Since $I - AA^\#$ is also nonzero, there exists a nonnegative vector w such that $(I - AA^\#)w$ is also nonzero (and nonnegative). Since v and $(I - AA^\#)w$ both lie in the same one-dimensional subspace, there exists $\beta \in \mathbb{R}$ such that $v = \beta(I - AA^\#)w$. If $\beta \geq 0$ then $v \geq 0$, whereas if $\beta \leq 0$ then $v \leq 0$. \square

COROLLARY 2.1. *Suppose that $E(0) \geq 0$, $P \geq 0$, and $P \in \mathcal{R}(A)$. Furthermore, assume that $\text{rank } A = n - 1$ and let $v \in \mathbb{R}^n$, $v \neq 0$, $v \geq 0$ satisfy $Av = 0$. Then the steady-state energy distribution E given by (2.10) has the form*

$$(2.14) \quad E = \beta v - A^\#P,$$

where $\beta = \|(I - AA^\#)E(0)\| / \|v\|$ and $\|\cdot\|$ denotes an arbitrary norm on \mathbb{R}^n .

Proof. Since A is singular there exists nonzero $v \in \mathcal{N}(A)$. Furthermore, since $\text{rank } A = n - 1$, it follows from Lemma 2.3 that either $v \geq 0$ or $-v \geq 0$. Without loss of generality, let v be chosen such that $v \geq 0$. Since $\text{rank } A = n - 1$, it follows that $\mathcal{N}(A)$ and thus $\mathcal{R}(I - AA^\#)$ are one dimensional. Thus there exists $\beta \geq 0$ such that $\beta v = (I - AA^\#)E(0)$. Note that β is necessarily nonnegative since v is nonzero and v and $(I - AA^\#)E(0)$ are both nonnegative vectors. Taking norms yields the given expression for β . \square

Remark 2.3. A sufficient condition for a singular M -matrix A to have rank $n - 1$ is for A to be irreducible (see [6, Thm. 6.4.16, p. 156]). In this case the nonnegative vector $v \in \mathcal{N}(A)$ actually has all positive components (see [6]).

As an application of Corollary 2.1 we consider the case in which $\sigma_{ii} = 0$, $i = 1, \dots, n$. Then $e^T A = 0$, which implies that $\text{rank } A \leq n - 1$. In this case it is easy to see

that when $P = 0$ the total system energy is conserved, since (2.8) implies $\mathbf{e}^T \dot{E}(t) = \mathbf{e}^T A E(t) = 0$. If we also assume that $A\mathbf{e} = 0$, we obtain the following result.

COROLLARY 2.2. *Suppose that $\sigma_{ii} = 0, i = 1, \dots, n, A\mathbf{e} = 0$, and $\text{rank } A = n - 1$. If $E(0) \geq 0$ and $P = 0$, then the steady-state energy distribution E given by (2.10) has the form*

$$(2.15) \quad E = \left[\frac{1}{n} \sum_{i=1}^n E_i(0) \right] \mathbf{e}.$$

Proof. Since $A\mathbf{e} = 0$, it follows from Corollary 2.1 and (2.14) that $E = \beta\mathbf{e}$, where (choosing the Euclidean norm in Corollary 2.1) $\beta = n^{-1/2}[E^T(0)(I - AA^\#)^T(I - AA^\#)E(0)]^{1/2}$. Next, since $A\mathbf{e} = A^T\mathbf{e} = 0$ and $\text{rank } A = n - 1$, it follows that A is an EP matrix ([61, p. 74]). Consequently, $AA^\#$ is symmetric and, in particular, $I - AA^\# = (1/n)\mathbf{e}\mathbf{e}^T$. This implies that $\beta = n^{-1}\mathbf{e}^T E(0)$, which yields (2.15). \square

The result (2.15) shows that under the stated assumptions each component of the steady-state energy vector is equal, that is, the steady-state energy is uniformly distributed over all states. This phenomenon is known as *equipartition of energy* [34], [41], [50].

Henceforth we consider the case in which A is nonsingular, that is, in which $-A$ is a nonsingular M -matrix. Numerous necessary and sufficient conditions for a Z -matrix to be a nonsingular M -matrix are given by [6, Thm. 6.2.3]. The following easily verified condition is sufficient but not necessary.

LEMMA 2.4. *If $\sigma_{ii} > 0, i = 1, \dots, n$, then $-A$ is a nonsingular M -matrix.*

Proof. If $\sigma_{ii} > 0, i = 1, \dots, n$, then $-A^T\mathbf{e} = [\sigma_{11} \dots \sigma_{nn}]^T \gg 0$. By [6, Condition (I₂₇), p. 136], $-A^T$, and hence $-A$, is a nonsingular M -matrix. \square

Next we examine the steady-state energy distribution E as a function of the coupling parameters $\sigma_{ij}, i \neq j$. Specifically, we wish to determine the steady-state energy distribution E in the limit of strong coupling, that is, as $\sigma_{ij} \rightarrow \infty, i \neq j$. To do this, define

$$A_\alpha \triangleq -D + \alpha C,$$

where the diagonal matrix D is defined by $D = \text{diag}(\sigma_{11}, \dots, \sigma_{nn})$ and the matrix C of coupling parameters is defined by

$$(2.16) \quad C_{ii} = - \sum_{\substack{j=1 \\ j \neq i}}^n \sigma_{ji}, \quad i = 1, \dots, n,$$

$$(2.17) \quad C_{ij} = \sigma_{ij}, \quad i \neq j, \quad i, j = 1, \dots, n.$$

In the notation of the Appendix,

$$(2.18) \quad D = \{\sigma\}, \quad C = -\text{vecd}^{-1}(\langle\sigma\rangle^T\mathbf{e}) + \langle\sigma\rangle = A + D,$$

where $\{\sigma\}$ and $\langle\sigma\rangle$ denote the diagonal and off-diagonal portions, respectively, of A . Note that $A = A_1$. Furthermore, note that if $\sigma_{ii} > 0, i = 1, \dots, n$, then $-A_\alpha$ is a nonsingular M -matrix for all $\alpha \geq 0$. For $P \geq 0$, let E_α denote the steady-state energy distribution with A replaced by A_α , that is,

$$(2.19) \quad E_\alpha = -A_\alpha^{-1}P.$$

Note that letting $\alpha \rightarrow \infty$ corresponds to letting $\sigma_{ij} \rightarrow \infty, i \neq j$. The following result provides an expression for $\lim_{\alpha \rightarrow \infty} E_\alpha$, which is the steady-state energy distribution in the limit of strong coupling.

PROPOSITION 2.4. *If $\sigma_{ii} > 0, i = 1, \dots, n$, then $E_\infty \triangleq \lim_{\alpha \rightarrow \infty} E_\alpha$ exists and is given by*

$$(2.20) \quad E_\infty = [D^{-1} - D^{-1}CD^{-1}(CD^{-1})^\#]P.$$

Proof. Since $\mathbf{e}^T CD^{-1} = 0$, it follows from [6, Exercise 6.4.14, p. 155] that $-CD^{-1}$ is a singular M -matrix with “property c .” Hence [6, Lemma 6.4.11, p. 153] implies that $\text{ind}(CD^{-1}) = 1$. From [61, Cor. 7.6.4], we obtain

$$\begin{aligned} E_\infty &= \lim_{\alpha \rightarrow \infty} [D - \alpha C]^{-1}P \\ &= D^{-1} \lim_{\beta \rightarrow 0} \beta[\beta I - CD^{-1}]^{-1}P \\ &= [D^{-1} - D^{-1}CD^{-1}(CD^{-1})^\#]P. \quad \square \end{aligned}$$

A minor variation of the proof of Proposition 2.4 shows that E_∞ can be written equivalently as either

$$(2.21) \quad E_\infty = [D^{-1} - D^{-1}CD^{-1/2}(D^{-1/2}CD^{-1/2})^\#D^{-1/2}]P$$

or

$$(2.22) \quad E_\infty = [D^{-1} - D^{-1}C(D^{-1}C)^\#D^{-1}]P.$$

The symmetry of the expression (2.21) will be useful in obtaining a more explicit expression for E_∞ when C is symmetric and has rank $n - 1$. The next result shows that in this case strong coupling leads to energy equipartition.

COROLLARY 2.3. *Assume that $\sigma_{ii} > 0, i = 1, \dots, n$, and suppose that C is symmetric and rank $C = n - 1$. Then E_∞ is given by*

$$(2.23) \quad E_\infty = \begin{pmatrix} \mathbf{e}^T P \\ \mathbf{e}^T D \mathbf{e} \end{pmatrix} \mathbf{e}.$$

Proof. For convenience define $\hat{C} \triangleq D^{-1/2}CD^{-1/2}$, which also has rank $n - 1$. Since C and \hat{C} are symmetric, it follows that $\hat{C}D^{1/2}\mathbf{e} = 0$. By decomposing \hat{C} it can be shown that $I - \hat{C}\hat{C}^\# = (\mathbf{e}^T D \mathbf{e})^{-1}D^{1/2}\mathbf{e}\mathbf{e}^T D^{1/2}$. Hence, using (2.21), we obtain

$$\begin{aligned} E_\infty &= D^{-1/2}[I - \hat{C}\hat{C}^\#]D^{-1/2}P \\ &= (\mathbf{e}^T D \mathbf{e})^{-1}D^{-1/2}D^{1/2}\mathbf{e}\mathbf{e}^T D^{1/2}D^{-1/2}P \\ &= \begin{pmatrix} \mathbf{e}^T P \\ \mathbf{e}^T D \mathbf{e} \end{pmatrix} \mathbf{e}. \quad \square \end{aligned}$$

3. Second-moment analysis of state space systems. In this section we consider an arbitrary asymptotically stable linear system subjected to additive white noise disturbances. The second-moment matrix of the state then satisfies a matrix Lyapunov differential equation. From this matrix differential equation, we then extract a vector differential equation for the diagonal elements of the second-moment matrix. These diagonal elements are the second moments of the individual states. This section relies heavily on Kronecker matrix algebra, which is summarized in the Appendix.

To begin, consider the state space differential equation

$$(3.1) \quad \dot{x}(t) = Fx(t) + Gw(t), \quad t \geq 0,$$

where $F \in \mathbb{C}^{n \times n}, G \in \mathbb{C}^{n \times d}, w(\cdot)$ is d -dimensional zero-mean stationary Gaussian white noise with intensity I_d , and $x(0)$ is Gaussian distributed with not-necessarily zero mean.

The second-moment matrix of $x(t)$ defined by $Q(t) \triangleq \mathbb{E}[x(t)x^*(t)] \in \mathbb{C}^{n \times n}$ satisfies the matrix Lyapunov differential equation [66, p. 101],

$$(3.2) \quad \dot{Q}(t) = FQ(t) + Q(t)F^* + V, \quad t \geq 0,$$

where $Q(0) = \mathbb{E}[x(0)x^*(0)]$ and $V \triangleq GG^*$. The solution $Q(t)$ to (3.2) is given explicitly by

$$(3.3) \quad Q(t) = e^{Ft}Q(0)e^{F^*t} + \int_0^t e^{Fs}Ve^{F^*s} ds, \quad t \geq 0,$$

which shows that $Q(t)$ is a (Hermitian) nonnegative-definite matrix.

Applying the vec operator [67], [68] to (3.2) and using (A.7) (see the Appendix) yields

$$(3.4) \quad \text{vec } \dot{Q}(t) = (\bar{F} \oplus F) \text{vec } Q(t) + \text{vec } V.$$

Next, we use the $n^2 \times n^2$ orthogonal permutation matrix U to rearrange the components of $\text{vec } Q(t)$ so that the diagonal elements of $Q(t)$ appear as the first n elements. Hence (3.4) implies

$$(3.5) \quad U \text{vec } \dot{Q}(t) = MU \text{vec } Q(t) + U \text{vec } V,$$

where M is defined by

$$(3.6) \quad M \triangleq U(\bar{F} \oplus F)U^{-1} = U(\bar{F} \oplus F)U^T.$$

Since $U = \begin{bmatrix} U_d \\ U_o \end{bmatrix}$, identities (A.13) and (A.14) imply

$$U \text{vec } Q(t) = \begin{bmatrix} U_d \text{vec } Q(t) \\ U_o \text{vec } Q(t) \end{bmatrix} = \begin{bmatrix} \text{vecd } Q(t) \\ \text{veco } Q(t) \end{bmatrix},$$

and similarly for $\text{vec } \dot{Q}(t)$ and $\text{vec } V$.

Next, defining

$$\begin{aligned} E(t) &\triangleq \text{vecd } Q(t), & P &\triangleq \text{vecd } V, \\ \hat{E}(t) &\triangleq \text{veco } Q(t), & \hat{P} &\triangleq \text{veco } V, \end{aligned}$$

(3.5) can be written as

$$(3.7) \quad \begin{bmatrix} \dot{E}(t) \\ \dot{\hat{E}}(t) \end{bmatrix} = M \begin{bmatrix} E(t) \\ \hat{E}(t) \end{bmatrix} + \begin{bmatrix} P \\ \hat{P} \end{bmatrix}.$$

Note that $E(t)$ and P are real and nonnegative, whereas $\hat{E}(t)$ and \hat{P} are generally complex. Furthermore, $Q(t)$ and V can be reconstructed from $E(t)$, $\hat{E}(t)$, P , and \hat{P} by means of

$$(3.8) \quad Q(t) = \text{vecd}^{-1}(E(t)) + \text{veco}^{-1}(\hat{E}(t)), \quad V = \text{vecd}^{-1}(P) + \text{veco}^{-1}(\hat{P}).$$

Next, partition M defined by (3.6) as

$$(3.9) \quad M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix},$$

where, using (3.6), the subblocks of M are given by

$$\begin{aligned} M_{11} &\triangleq U_d(\bar{F} \oplus F)U_d^T, & M_{12} &\triangleq U_d(\bar{F} \oplus F)U_o^T, \\ M_{21} &\triangleq U_o(\bar{F} \oplus F)U_d^T, & M_{22} &\triangleq U_o(\bar{F} \oplus F)U_o^T. \end{aligned}$$

Using (A.11) and (A.17)–(A.20), M_{11} , M_{12} , M_{21} , and M_{22} can be simplified somewhat as

$$(3.10) \quad M_{11} = 2 \operatorname{Re} \{F\}, \quad M_{12} = U_d(\langle \bar{F} \rangle \oplus \langle F \rangle)U_d^T,$$

$$(3.11)$$

$$M_{21} = U_o(\langle \bar{F} \rangle \oplus \langle F \rangle)U_d^T, \quad M_{22} = U_o(\{\bar{F}\} \oplus \{F\})U_o^T + U_o(\langle \bar{F} \rangle \oplus \langle F \rangle)U_o^T,$$

where $\{F\}$ and $\langle F \rangle$ denote the diagonal and off-diagonal portions of F , respectively. Note that M_{11} is real and diagonal and that the term $U_o(\{\bar{F}\} \oplus \{F\})U_o^T$ appearing in M_{22} is diagonal.

We now wish to eliminate $\hat{E}(t)$ from (3.7) to obtain an equation solely in terms of $E(t)$. Hence solving for $\hat{E}(t)$ and substituting this expression into the equation for $\dot{E}(t)$ with $\hat{E}(0) = 0$ and $\hat{P} = 0$ yields the integro-differential equation

$$(3.12) \quad \dot{E}(t) = M_{11}E(t) + M_{12} \int_0^t e^{M_{22}(t-s)} M_{21}E(s) ds + P.$$

Again, using (3.7), it follows that the solution to (3.12) is given explicitly by

$$(3.13) \quad E(t) = [I_n \ 0]e^{Mt} \begin{bmatrix} I_n \\ 0 \end{bmatrix} E(0) + [I_n \ 0] \int_0^t e^{Ms} ds \begin{bmatrix} I_n \\ 0 \end{bmatrix} P.$$

Since $E(t)$ is nonnegative if $E(0)$ and P are nonnegative, we expect the coefficients of $E(0)$ and P in (3.13) to be nonnegative matrices. This is illustrated by the following result which provides explicit expressions for these matrices.

PROPOSITION 3.1. *The following identities are satisfied:*

$$(3.14) \quad [I_n \ 0]e^{Mt} \begin{bmatrix} I_n \\ 0 \end{bmatrix} = e^{Ft} \circ e^{\bar{F}t},$$

$$(3.15) \quad [I_n \ 0] \int_0^t e^{Ms} ds \begin{bmatrix} I_n \\ 0 \end{bmatrix} = \int_0^t e^{Fs} \circ e^{\bar{F}s} ds.$$

Proof. From (3.6) and (A.8) it follows that

$$\begin{aligned} [I_n \ 0]e^{Mt} \begin{bmatrix} I_n \\ 0 \end{bmatrix} &= [I_n \ 0]Ue^{(\bar{F} \oplus F)t}U^T \begin{bmatrix} I_n \\ 0 \end{bmatrix} \\ &= U_d e^{(\bar{F} \oplus F)t} U_d^T \\ &= U_d (e^{\bar{F}t} \otimes e^{Ft}) U_d^T \\ &= e^{\bar{F}t} \circ e^{Ft}, \end{aligned}$$

where the last step follows from (A.11). Integrating (3.14) over $[0, t]$ yields (3.15). □

From (3.14), we obtain the following result.

COROLLARY 3.1. *The following identities are satisfied:*

$$(3.16) \quad M_{12}M_{21} = 2F \circ \bar{F} + 2 \operatorname{Re} \{F^2\} - 4(\operatorname{Re} \{F\})^2,$$

$$(3.17) \quad \begin{aligned} M_{12}M_{22}M_{21} &= 2 \operatorname{Re} \{F^3\} - 8 \operatorname{Re} \{F\} \operatorname{Re} \{F^2\} + 8(\operatorname{Re} \{F\})^3 \\ &\quad + 6 \operatorname{Re} (F \circ \bar{F}^2) - 4 \operatorname{Re} \{F\}(F \circ \bar{F}) - 4(F \circ \bar{F}) \operatorname{Re} \{F\}. \end{aligned}$$

Proof. First note that for $t \rightarrow 0$

$$[I_n \ 0]e^{Mt} \begin{bmatrix} I_n \\ 0 \end{bmatrix} = I + M_{11}t + \frac{1}{2}(M_{11}^2 + M_{12}M_{21})t^2 + \frac{1}{6}(M_{11}^3 + M_{11}M_{12}M_{21} + M_{12}M_{21}M_{11} + M_{12}M_{22}M_{21})t^3 + O(t^4),$$

while

$$\begin{aligned} e^{Ft} \circ e^{\bar{F}t} &= (I + Ft + \frac{1}{2}F^2t^2 + \frac{1}{6}F^3t^3 + O(t^4)) \circ (I + \bar{F}t + \frac{1}{2}\bar{F}^2t^2 + \frac{1}{6}\bar{F}^3t^3 + O(t^4)) \\ &= I + \{F + \bar{F}\}t + (\frac{1}{2}\{F^2 + \bar{F}^2\} + F \circ \bar{F})t^2 \\ &\quad + (\frac{1}{3} \operatorname{Re} \{F^3\} + \operatorname{Re} (F \circ \bar{F}^2))t^3 + O(t^4). \end{aligned}$$

Equating terms of $O(t^2)$ and $O(t^3)$ yields (3.16) and (3.17). \square

COROLLARY 3.2. *The matrix $M_{12}M_{21}$ is essentially nonnegative.*

Proof. The result follows from the fact that $\langle M_{12}M_{21} \rangle = 2\langle F \circ \bar{F} \rangle \geq 0$. \square

Using expressions (3.14) and (3.15), (3.13) for $E(t)$ can be written as

$$(3.18) \quad E(t) = e^{Ft} \circ e^{\bar{F}t} E(0) + \int_0^t e^{Fs} \circ e^{\bar{F}s} dsP.$$

For comparison, let us recall the solution (2.9) to the compartmental model (2.8) given by

$$(3.19) \quad E(t) = e^{At} E(0) + \int_0^t e^{As} dsP.$$

These models, that is, (3.18) and (3.19), will coincide if and only if

$$(3.20) \quad e^{At} = e^{Ft} \circ e^{\bar{F}t}, \quad t \geq 0.$$

In general, however, there does not exist a matrix A satisfying (3.19) for the obvious reason that $e^{Ft} \circ e^{\bar{F}t}$ involves more spectral content than can be provided by the exponential of a single $n \times n$ matrix. It is easy to see that there exists a matrix A such that (3.19) and (3.20) coincide if and only if F is diagonal, in which case $A = F + \bar{F}$. To proceed, let us consider the steady-state problem. To guarantee that $\lim_{t \rightarrow \infty} E(t)$ exists, we shall assume that F is semistable. The following result will be useful.

LEMMA 3.1. *If F is semistable, then M is semistable.*

Proof. Since $e^{Mt} = U(e^{\bar{F}t} \otimes e^{Ft})U^T$, the existence of $\lim_{t \rightarrow \infty} e^{Ft}$ implies the existence of $\lim_{t \rightarrow \infty} e^{Mt}$. \square

PROPOSITION 3.2. *Suppose that F is semistable and assume that $P \in \mathcal{N}(I_n - U_d(\bar{F} \oplus F)(\bar{F} \oplus F)^{\#}U_d^T)$. Then $E \triangleq \lim_{t \rightarrow \infty} E(t)$ exists and is given by*

$$(3.21) \quad E = (I - FF^{\#}) \circ (I - \bar{F}\bar{F}^{\#})E(0) - U_d(\bar{F} \oplus F)^{\#}U_d^T P.$$

Proof. The first term in (3.21) follows from (iv) of Lemma 2.2. Since $\operatorname{ind}(M) = 1$, we have (using (vi) of Lemma 2.2)

$$\begin{aligned} \int_0^t e^{Fs} \circ e^{\bar{F}s} dsP &= [I_n \ 0] \int_0^t e^{Ms} ds \begin{bmatrix} I_n \\ 0 \end{bmatrix} P \\ &= [I_n \ 0] M^{\#}(e^{Mt} - I) \begin{bmatrix} I_n \\ 0 \end{bmatrix} P + [I_n \ 0](I - MM^{\#}) \begin{bmatrix} I_n \\ 0 \end{bmatrix} Pt. \end{aligned}$$

Since $[I_n \ 0](I - MM^\#)[I_n^T; 0] = I_n - U_d(\bar{F} \oplus F)(\bar{F} \oplus F)^\# U_d^T$, the term linear in t is zero by assumption. Consequently, as $t \rightarrow \infty$,

$$\int_0^t e^{Fs} \circ e^{\bar{F}s} ds P \rightarrow -[I_n \ 0]M^\# \begin{bmatrix} I_n \\ 0 \end{bmatrix} P,$$

which is equal to $-U_d(\bar{F} \oplus F)^\# U_d^T P$. \square

When the rank of F is $n - 1$, some simplification is possible.

COROLLARY 3.3. *Let F and P be as in Proposition 3.2. Furthermore, assume that $\text{rank } F = n - 1$ and let $v \in \mathbb{C}^n, v \neq 0$, satisfy $Fv = 0$. Then E is given by*

$$(3.22) \quad E = \left(\frac{(v \circ \bar{v})^T E(0)}{(v^*v)^2} \right) v \circ \bar{v} - U_d(\bar{F} \oplus F)^\# U_d^T P.$$

Proof. Since $\text{rank}(I - FF^\#) = 1$, it follows that $I - FF^\# = wy^*$ for some nonzero $w, y \in \mathbb{C}^n$. Hence $v = (y^*v)w, y = (y^*v/v^*v)(I - FF^\#)^*v$, and $I - FF^\# = (v^*v)^{-1}vv^*(I - FF^\#)$. Using (A.10) in (3.21) now yields (3.22). \square

4. Steady-state compartmental modeling of the diagonal system. In the previous section it was shown that the evolution of the diagonal portion of the second-moment matrix cannot generally be modeled by means of an n th-order state space system. Hence we now focus our attention on the steady-state solution to the diagonal system. Our goal is to determine conditions under which the steady-state energy distribution of the diagonal system coincides with the steady-state energy distribution of a compartmental model. Henceforth (and without further notice) we assume that F is asymptotically stable, that is, every eigenvalue of F has negative real part.

Since F is asymptotically stable, $Q \triangleq \lim_{t \rightarrow \infty} Q(t)$ exists, is nonnegative definite, and is given by

$$(4.1) \quad Q = \int_0^\infty e^{Fs} V e^{F^*s} ds,$$

which is the unique solution to the algebraic Lyapunov equation

$$(4.2) \quad 0 = FQ + QF^* + V.$$

Note that Q is independent of $Q(0)$. Furthermore, since $\bar{F} \oplus F$ is asymptotically stable [67], [68], M is asymptotically stable so that (3.13) can be written as

$$(4.3) \quad E(t) = [I_n \ 0]e^{Mt} \begin{bmatrix} I_n \\ 0 \end{bmatrix} E(0) + [I_n \ 0]M^{-1}(e^{Mt} - I) \begin{bmatrix} I_n \\ 0 \end{bmatrix} P.$$

Now letting $t \rightarrow \infty$ in (3.7) yields

$$(4.4) \quad \begin{bmatrix} E \\ \hat{E} \end{bmatrix} = -M^{-1} \begin{bmatrix} P \\ \hat{P} \end{bmatrix},$$

where $E \triangleq \lim_{t \rightarrow \infty} E(t)$ and $\hat{E} \triangleq \lim_{t \rightarrow \infty} \hat{E}(t)$. For convenience, partition M^{-1} as

$$(4.5) \quad M^{-1} = \begin{bmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{bmatrix},$$

where

$$\begin{aligned} N_{11} &\triangleq U_d(\bar{F} \oplus F)^{-1} U_d^T, & N_{12} &\triangleq U_d(\bar{F} \oplus F)^{-1} U_o^T, \\ N_{21} &\triangleq U_o(\bar{F} \oplus F)^{-1} U_d^T, & N_{22} &\triangleq U_o(\bar{F} \oplus F)^{-1} U_o^T. \end{aligned}$$

Next, letting $t \rightarrow \infty$ in (4.3) yields

$$(4.6) \quad N_{11} = - \int_0^\infty e^{Ft} \circ e^{\bar{F}t} dt,$$

which shows that $-N_{11}$ is a (real) nonnegative matrix. Finally, if $\bar{P} = 0$, then (4.4) implies that E is given by

$$(4.7) \quad E = -N_{11}P.$$

Returning to (3.18), the assumption that F is asymptotically stable implies that $E = \lim_{t \rightarrow \infty} E(t)$ exists for all $E(0)$ and P . Hence we consider the case in which A is also asymptotically stable so that $E = \lim_{t \rightarrow \infty} E(t)$ also exists for $E(t)$ given by (3.19). In this case, the steady-state solution to (3.19) is given by (2.11), that is,

$$(4.8) \quad E = -A^{-1}P.$$

Requiring that the steady-state values given by (4.7) and (4.8) be equal yields

$$(4.9) \quad A^{-1} = N_{11}.$$

The matrix A given by (4.9) will be called the *derived* model. However, for the derived model to exist, N_{11} must be nonsingular. The following result addresses this question.

PROPOSITION 4.1. N_{11} is nonsingular if and only if M_{22} is nonsingular. In this case

$$(4.10) \quad N_{11}^{-1} = M_{11} - M_{12}M_{22}^{-1}M_{21},$$

$$(4.11) \quad M_{22}^{-1} = N_{22} - N_{21}N_{11}^{-1}N_{12}.$$

Proof. The result follows immediately from $M^{-1}M = I_n$. \square

COROLLARY 4.1. Suppose that M_{22} is nonsingular. Then $M_{12}M_{22}^{-1}M_{21}$ is real.

Proof. From (4.10) it follows that $M_{12}M_{22}^{-1}M_{21} = M_{11} - N_{11}^{-1}$. Since M_{11} and N_{11}^{-1} are real (in fact, $-N_{11}$ is nonnegative), $M_{12}M_{22}^{-1}M_{21}$ is also real. \square

Hence if M_{22} is nonsingular, then (4.9) and (4.10) imply that A is given by

$$(4.12) \quad A = M_{11} - M_{12}M_{22}^{-1}M_{21}.$$

It remains to be shown, however, that A given by (4.12) is asymptotically stable and represents the dynamics of a compartmental model as defined by (2.4), (2.5). For convenience in discussing (4.12) define

$$(4.13) \quad \mu \triangleq -M_{11}, \quad \mathcal{P} \triangleq M_{12}M_{22}^{-1}M_{21}$$

so that (4.12) can be written as

$$(4.14) \quad A = -(\mu + \mathcal{P}).$$

The key to analyzing (4.14) is to exploit the structure of M_{22}^{-1} . To facilitate our analysis, decompose F as $F = \{F\} + \langle F \rangle$ so that M_{22} can be written as

$$(4.15) \quad M_{22} = L_d + L_o,$$

where

$$L_d \triangleq U_o(\{\bar{F}\} \oplus \{F\})U_o^T, \quad L_o \triangleq U_o(\langle \bar{F} \rangle \oplus \langle F \rangle)U_o^T.$$

Note that L_d and L_o depend upon the diagonal and off-diagonal portions of F , respectively. When L_d and M_{22} are nonsingular, we use the decomposition (4.15) and consider the identity

$$(4.16) \quad M_{22}^{-1} = L_d^{-1} - L_d^{-1}L_oM_{22}^{-1},$$

which implies that

$$(4.17) \quad M_{12}M_{22}^{-1}M_{21} = M_{12}L_d^{-1}M_{21} - M_{12}L_d^{-1}L_oM_{22}^{-1}M_{21}.$$

Let us rewrite (4.17) as

$$(4.18) \quad \mathcal{P} = \mathcal{P}_0 + \mathcal{R}_0,$$

where

$$(4.19) \quad \mathcal{P}_0 \triangleq M_{12}L_d^{-1}M_{21}, \quad \mathcal{R}_0 \triangleq -M_{12}L_d^{-1}L_oM_{22}^{-1}M_{21}.$$

In (4.18), \mathcal{P}_0 can be viewed as the zeroth-order term in an expansion of \mathcal{P} while \mathcal{R}_0 is the corresponding remainder. To evaluate \mathcal{P}_0 , define the Hermitian matrix $\Gamma \in \mathbb{C}^{n \times n}$ by

$$(4.20) \quad \Gamma_{ij} \triangleq \frac{1}{\bar{F}_{ii} + F_{jj}}, \quad i, j = 1, \dots, n.$$

PROPOSITION 4.2. *Suppose that L_d is nonsingular. Then*

$$(4.21) \quad \mathcal{P}_0 = 2 \operatorname{Re} [\{ \langle \Gamma \cdot F \rangle F \} + \langle \Gamma \cdot F \cdot \bar{F} \rangle].$$

Proof. First note that

$$L_d^{-1} = U_o \left[\sum_{\substack{i,j=1 \\ i \neq j}}^n \Gamma_{ij} \mathcal{E}_{ii} \otimes \mathcal{E}_{jj} \right] U_o^T.$$

Then using (A.4), (A.11), (A.13), and $\bar{\Gamma}_{ij} = \Gamma_{ji}$, we have

$$\begin{aligned} \mathcal{P}_0 &= U_d(\bar{F} \oplus F) \left[\sum_{\substack{i,j=1 \\ i \neq j}}^n \Gamma_{ij} \mathcal{E}_{ii} \otimes \mathcal{E}_{jj} \right] (\bar{F} \oplus F) U_d^T \\ &= \sum_{\substack{i,j=1 \\ i \neq j}}^n \Gamma_{ij} [(F \mathcal{E}_{jj} F) \cdot \mathcal{E}_{ii} + (\bar{F} \mathcal{E}_{ii} \bar{F}) \cdot \mathcal{E}_{jj} + (\mathcal{E}_{jj} F) \cdot (\bar{F} \mathcal{E}_{ii}) + (\mathcal{E}_{ii} \bar{F}) \cdot (F \mathcal{E}_{jj})] \\ &= \sum_{\substack{i,j=1 \\ i \neq j}}^n \Gamma_{ij} [F_{ij} F_{ji} \mathcal{E}_{ii} + \bar{F}_{ji} \bar{F}_{ij} \mathcal{E}_{jj} + F_{ji} \bar{F}_{ji} \mathcal{E}_{ji} + F_{ij} \bar{F}_{ij} \mathcal{E}_{ij}] \\ &= 2 \operatorname{Re} \sum_{\substack{i,j=1 \\ i \neq j}}^n [\Gamma_{ij} F_{ij} F_{ji} \mathcal{E}_{ii} + \Gamma_{ij} F_{ij} \bar{F}_{ij} \mathcal{E}_{ij}] \\ &= 2 \operatorname{Re} \left[\sum_{i=1}^n \sum_{\substack{j=1 \\ j \neq i}}^n (\Gamma \cdot F)_{ij} F_{ji} \mathcal{E}_{ii} + \sum_{\substack{i,j=1 \\ i \neq j}}^n (\Gamma \cdot F \cdot \bar{F})_{ij} \mathcal{E}_{ij} \right] \\ &= 2 \operatorname{Re} [\{ \langle \Gamma \cdot F \rangle F \} + \langle \Gamma \cdot F \cdot \bar{F} \rangle]. \quad \square \end{aligned}$$

COROLLARY 4.2. *Suppose that $\{F\}$ is asymptotically stable. Then L_d is nonsingular and \mathcal{P}_0 is a Z-matrix. If, in addition, F has no zero off-diagonal elements, then \mathcal{P}_0 is essentially negative (has negative off-diagonal elements).*

Proof. If $\{F\}$ is asymptotically stable, then L_d is nonsingular. The result now follows from the fact that for $i \neq j$

$$(\mathcal{P}_0)_{ij} = 2 |F_{ij}|^2 \operatorname{Re} (F_{ii} + F_{jj}) / |\bar{F}_{ii} + F_{jj}|^2 \leq 0.$$

If, in addition, $F_{ij} \neq 0$, then $(\mathcal{P}_0)_{ij} < 0$. □

Next let us define

$$(4.22) \quad F_\alpha = \{F\} + \alpha \langle F \rangle,$$

where $\{F\}$ and $\alpha \langle F \rangle$ are diagonal and off-diagonal matrices, respectively, and α is a positive number. The scalar α in (4.22) allows us to adjust the strength of the off-diagonal coupling in F_α . When F is replaced by F_α , derived quantities such as M_{22} and \mathcal{P}_0 are written as $M_{22\alpha}$ and $\mathcal{P}_{0\alpha}$. Consequently, (4.12) becomes

$$(4.23) \quad A_\alpha = M_{11} - M_{12\alpha} M_{22\alpha}^{-1} M_{21\alpha}.$$

We thus have the following result for the case of weak coupling, that is, for $\alpha \approx 0$.

COROLLARY 4.3. *Suppose that $\{F\}$ is asymptotically stable and F has no zero off-diagonal elements. Then there exists $\alpha_0 > 0$ such that F_α is asymptotically stable, $M_{22\alpha}$ is nonsingular, and \mathcal{P}_α is essentially negative for all $\alpha \in (0, \alpha_0)$.*

Proof. By Corollary 4.2, $\mathcal{P}_{0\alpha} = M_{12\alpha} L_d^{-1} M_{21\alpha}$ is essentially negative for all $\alpha > 0$. Furthermore, it follows from (3.10) and (3.11) that $\mathcal{P}_{0\alpha} = O(\alpha^2)$ as $\alpha \rightarrow 0$. Thus if α is sufficiently small, then F_α is asymptotically stable and $M_{22\alpha} = L_d + \alpha L_o$ is nonsingular. Consequently, $\mathcal{R}_{0\alpha} = O(\alpha^3)$. The result now follows from the fact that $\mathcal{P}_\alpha = \mathcal{P}_{0\alpha} + \mathcal{R}_{0\alpha}$. □

THEOREM 4.1. *Suppose that $\{F\}$ is asymptotically stable and F has no zero off-diagonal elements. Then there exists $\alpha_0 > 0$ such that $-A_\alpha$ is a nonsingular M -matrix for all $\alpha \in [0, \alpha_0)$.*

Proof. Let $\alpha \in [0, \alpha_0)$, where α_0 is given by Corollary 4.3. Since by (4.14) $-\langle A_\alpha \rangle = \langle \mathcal{P}_\alpha \rangle$, it follows from Corollary 4.3 that $-A_\alpha$ is a Z -matrix. Furthermore, by (4.6) and (4.9), $-A_\alpha^{-1} = \int_0^\infty e^{F_\alpha t} \circ e^{F_\alpha t} dt$ is nonnegative. Hence it follows from [6, p. 137], that $-A_\alpha$ is a nonsingular M -matrix. □

COROLLARY 4.4. *Under the assumptions of Theorem 4.1, A_α is asymptotically stable for all $\alpha \in [0, \alpha_0)$.*

Proof. By [6, p. 135], each eigenvalue of $-A_\alpha$ has a positive real part. Hence A_α is asymptotically stable. □

The remainder of this section is devoted to further analysis of the properties of \mathcal{P} . The following result gives an alternative sufficient condition for M_{22} to be asymptotically stable and hence nonsingular.

PROPOSITION 4.3. *If F is upper triangular, then M_{22} is asymptotically stable.*

Proof. The result follows from the fact that L_d is asymptotically stable and L_o is strictly upper triangular. □

PROPOSITION 4.4. *Suppose that M_{22} is nonsingular. If F is symmetric (but not necessarily either real or Hermitian), then \mathcal{P} is symmetric. If, in addition, \mathcal{P} is a Z -matrix, then A defined by (4.14) is negative definite.*

Proof. If F is symmetric, then so are $\langle F \rangle$ and $\langle \bar{F} \rangle$. The result is now immediate. □

Next, we consider the case in which $\langle F \rangle$ is skew-Hermitian. This case arises frequently in applications in which the modal coupling is energy conservative.

PROPOSITION 4.5. *Suppose that M_{22} is nonsingular. If $\langle F \rangle$ is skew-Hermitian, then*

$$(4.24) \quad \mathcal{P}\mathbf{e} = \mathcal{P}^T\mathbf{e} = 0.$$

If, in addition, $\text{Re} \langle F \rangle = 0$, then \mathcal{P} is symmetric.

Proof. Using the fact that $\text{vecd } I_n = \mathbf{e}$ along with (A.14) and (A.16) yields

$$\begin{aligned} (\langle \bar{F} \rangle \oplus \langle F \rangle)U_d^T\mathbf{e} &= (\langle \bar{F} \rangle \oplus \langle F \rangle)U_d^T \text{vecd } I_n \\ &= (\langle \bar{F} \rangle \oplus \langle F \rangle) \text{vec } I_n \\ &= \text{vec} (\langle F \rangle + \langle \bar{F} \rangle^T) \\ &= 0, \end{aligned}$$

which along with (3.11) and (4.13) implies that $\mathcal{P}\mathbf{e} = 0$. A similar argument shows that $\mathcal{P}^T\mathbf{e} = 0$. If $\text{Re} \langle F \rangle = 0$, then $\langle F \rangle = j\hat{F}$, where \hat{F} is real. Since $\langle F \rangle$ is skew-Hermitian, it follows that \hat{F} is symmetric. Consequently, $\langle F \rangle$ is symmetric, which implies that F is symmetric. Now by Proposition 4.4, \mathcal{P} is symmetric. \square

5. Compartmental modeling of state space systems. In this section we relate the steady-state second-moment analysis of § 4 to the compartmental model discussed in § 2.

If $-A$ is a nonsingular M -matrix (assuming M_{22} is nonsingular), it follows from property (M_{36}) [6, p. 137], that there exists a diagonal matrix $D = \text{diag}(d_1, \dots, d_n)$ with positive diagonal elements $d_i > 0, i = 1, \dots, n$, such that $D(-A)D^{-1}$ is strictly diagonally dominant, that is,

$$(5.1) \quad -A_{ii} > \sum_{\substack{j=1 \\ j \neq i}}^n (d_j/d_i)A_{ji}.$$

Note that $-A_{ii}$ is positive since a nonsingular M -matrix has positive diagonal elements. Now define $\hat{A} \triangleq DAD^{-1}$ and note that $-\hat{A}$ is also a nonsingular M -matrix. To show that \hat{A} has the form of a compartmental model, define

$$(5.2) \quad \sigma_{ii} \triangleq -A_{ii} - \sum_{\substack{j=1 \\ j \neq i}}^n (d_j/d_i)A_{ji}, \quad i = 1, \dots, n,$$

$$(5.3) \quad \sigma_{ij} \triangleq (d_i/d_j)A_{ij}, \quad i \neq j, \quad i, j = 1, \dots, n.$$

With (5.3) we can rewrite (5.2) as

$$(5.4) \quad \sigma_{ii} = -A_{ii} - \sum_{\substack{j=1 \\ j \neq i}}^n \sigma_{ji}.$$

Since $\hat{A}_{ij} = (d_i/d_j)A_{ij}$, it follows that

$$(5.5) \quad \hat{A}_{ii} = \sum_{j=1}^n \sigma_{ji}, \quad i = 1, \dots, n,$$

$$(5.6) \quad \hat{A}_{ij} = \sigma_{ij}, \quad i \neq j, \quad i, j = 1, \dots, n,$$

which verifies (2.4), (2.5) with A replaced by \hat{A} .

Next, we introduce the scaled energy states $E_s \triangleq DE$ and scaled power input $P_s \triangleq DP$ so that (4.8) becomes

$$(5.7) \quad 0 = \hat{A}E_s + P_s.$$

With this scaling and the definition of \hat{A} , (5.7) has the form of a steady-state compartmental model as given by (2.12).

Remark 5.1. Consider the energy conservative case in which $\langle F \rangle$ is skew-Hermitian so that (4.23) holds. Then the row and column sums of \mathcal{P} are zero. If \mathcal{P} is also a Z -matrix, then no scaling is required (that is, $D = I$ suffices) to obtain a steady-state compartmental model.

6. Conclusion. Compartmental models are widely used to represent the dynamics of systems involving the exchange of inherently nonnegative quantities such as mass or energy. In this paper we summarized some of the key properties of these models and characterized their steady-state energy distribution. In addition, conditions were given under which the steady-state energy distribution tends toward equipartition in the limit of strong off-diagonal coupling. We then considered arbitrary state space models with additive white noise disturbance and obtained an equation that governs the evolution of the nonnegative diagonal system. The steady-state limit of this diagonal system was then examined for its relationship to steady-state compartmental models. The key step in this regard was to show that the coefficient matrix is a Z -matrix, that is, has nonpositive off-diagonal elements. It was shown that if the off-diagonal coupling is sufficiently weak, then (up to a positive scaling) the diagonal system does in fact have the form of a compartmental model. Conditions under which the diagonal system is a compartmental model in the case of strong coupling remain an area for future research.

Appendix. Kronecker matrix algebra. In this Appendix we review some basic definitions and identities from Kronecker matrix algebra. Our main references are [67] and [68]. We also introduce several specialized definitions that are specific to this paper.

For $A \in \mathbb{C}^{n \times m}$, let $\text{col}_i(A)$ denote the i th column of A and define the vec and vec^{-1} operators by

$$\text{vec } A \triangleq \begin{bmatrix} \text{col}_1(A) \\ \vdots \\ \text{col}_m(A) \end{bmatrix} \in \mathbb{C}^{nm}, \quad \text{vec}^{-1}(\text{vec } A) \triangleq A.$$

For $A \in \mathbb{C}^{n \times m}$ and $B \in \mathbb{C}^{p \times q}$, the Kronecker product of A and B is defined by

$$A \otimes B \triangleq \begin{bmatrix} A_{11}B & A_{12}B & \cdots & A_{1m}B \\ A_{21}B & A_{22}B & \cdots & A_{2m}B \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1}B & A_{n2}B & \cdots & A_{nm}B \end{bmatrix} \in \mathbb{R}^{np \times mq},$$

while for $A \in \mathbb{C}^{n \times n}$ and $B \in \mathbb{C}^{m \times m}$ the Kronecker sum of A and B is defined by

$$A \oplus B \triangleq A \otimes I_m + I_n \otimes B \in \mathbb{C}^{nm \times nm}.$$

For compatible complex matrices A, B, C, D , the following identities hold:

$$(A.1) \quad (A + B) \otimes C = A \otimes C + B \otimes C,$$

$$(A.2) \quad A \otimes (B + C) = A \otimes B + A \otimes C,$$

$$(A.3) \quad (A \otimes B)^T = A^T \otimes B^T, \quad (A \oplus B)^T = A^T \oplus B^T,$$

$$(A.4) \quad (A \otimes B)(C \otimes D) = (AC) \otimes (BD),$$

$$(A.5) \quad (A \otimes B)^{-1} = A^{-1} \otimes B^{-1},$$

$$(A.6) \quad \text{vec } ABC = (C^T \otimes A) \text{vec } B,$$

$$(A.7) \quad \text{vec } (AB + BC) = (C^T \oplus A) \text{vec } B,$$

$$(A.8) \quad e^{A \oplus B} = e^A \otimes e^B,$$

$$(A.9) \quad (A \otimes B) \circ (C \otimes D) = (A \circ C) \otimes (B \circ D).$$

If $w, y \in \mathbb{C}^n$ and $x, z \in \mathbb{C}^m$, then

$$(A.10) \quad (wx^T) \circ (yz^T) = (w \circ y)(x \circ z)^T.$$

Next, let e_i denote the i th column of the $n \times n$ identity matrix, where the dimension n is determined by context, and define $\mathcal{E}_{rs} \triangleq e_r e_s^T$, which is the not-necessarily square matrix whose (r, s) element is 1 and whose remaining elements are all 0. Now define the $n \times n^2$ matrix

$$U_d \triangleq [\mathcal{E}_{11} \mathcal{E}_{22} \cdots \mathcal{E}_{nn}] = \sum_{i=1}^n e_i^T \otimes \mathcal{E}_{ii}.$$

Furthermore, letting I_{ji} denote the $(n - 1) \times n$ matrix obtained by deleting the i th row of the $n \times n$ identity matrix, define the $(n^2 - n) \times n^2$ matrix

$$U_o \triangleq \begin{bmatrix} I_{j1} & & & \\ & I_{j2} & 0 & \\ & 0 & \ddots & \\ & & & I_{jn} \end{bmatrix} = \sum_{i=1}^n \mathcal{E}_{ii} \otimes I_{ji}.$$

If $A, B \in \mathbb{C}^{n \times n}$, then [69] and [70]

$$(A.11) \quad U_d(A \otimes B)U_d^T = U_d(B \otimes A)U_d^T = A \circ B.$$

Note that U_d and U_o satisfy the identities

$$(A.12) \quad U_d U_d^T = I_n, \quad U_d U_o^T = \mathbf{0}_{n \times (n^2 - n)}, \quad U_o U_o^T = I_{n^2 - n},$$

$$(A.13) \quad U_o^T U_o = \sum_{\substack{i,j=1 \\ i \neq j}}^n \mathcal{E}_{ii} \otimes \mathcal{E}_{jj}.$$

Hence the matrix $U \in \mathbb{R}^{n^2 \times n^2}$ defined by

$$U \triangleq \begin{bmatrix} U_d \\ U_o \end{bmatrix}$$

satisfies $U^T = U^{-1}$; that is, U is an orthogonal (but not symmetric) permutation matrix.

For a square matrix $A \in \mathbb{C}^{n \times n}$, let $\{A\}$ and $\langle A \rangle$ denote the diagonal and off-diagonal portions of A , respectively. That is, $\{A\}$ is the diagonal matrix defined by

$$\{A\} \triangleq I \circ A,$$

and $\langle A \rangle$ is the off-diagonal matrix defined by

$$\langle A \rangle \triangleq A - \{A\}.$$

Next, as in [67], let $\text{vecd } A$ denote the n -vector comprised of the diagonal elements of A , that is,

$$\text{vecd } A \triangleq \begin{bmatrix} A_{11} \\ \vdots \\ A_{nn} \end{bmatrix} = \{A\} \mathbf{e}, \quad \text{vecd}^{-1}(\text{vecd } A) \triangleq \{A\},$$

where $\mathbf{e} \triangleq [1 \ 1 \ \cdots \ 1]^T$, and let $\text{veco } A$ denote the $(n^2 - n)$ -vector comprised of the off-diagonal elements of A ordered in accordance with $\text{vec } A$. Define also $\text{veco}^{-1}(\text{veco } A) \triangleq \langle A \rangle$. The above-defined operators satisfy the following identities:

(A.14) $\text{vecd } A = U_d \text{vec } A = \text{vecd } \{A\} = U_d \text{vec } \{A\},$

(A.15) $\text{veco } A = U_o \text{vec } A = \text{veco } \langle A \rangle = U_o \text{vec } \langle A \rangle,$

(A.16) $\text{vec } \{A\} = U_d^T \text{vecd } A, \quad \text{vec } \langle A \rangle = U_o^T \text{veco } A.$

Finally, if $A, B \in \mathbb{C}^{n \times n}$, it is useful to note that

(A.17) $\{A \oplus B\} = \{A\} \oplus \{B\}, \quad \langle A \oplus B \rangle = \langle A \rangle \oplus \langle B \rangle,$

(A.18) $A \oplus B = \{A\} \oplus \{B\} + \langle A \rangle \oplus \langle B \rangle,$

(A.19) $U_d(A \oplus B)U_d^T = \{A + B\}, \quad U_o\{A \oplus B\}U_d^T = 0,$

(A.20) $U_o(A \oplus B)U_d^T = U_o(\langle A \rangle \oplus \langle B \rangle)U_d^T.$

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