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A Phenomenological Calculus for Complex Systems

I. W. RICHARDSON, A. H. LOUIE AND S. SWAMINATHAN

Departments of Physiology and Biophysics, and Mathematics, Dalhousie University, Halifax, Nova Scotia, Canada B3H 4H7

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The difficulties in framing and solving dynamical equations encompassing the detailed interactions of complex biological systems are legion. As an alternative to comprehensive system dynamics, a calculus is derived which phenomenologically relates generalized causes to their resultant dynamical effects. A complex system is divided into distinct, interacting subsystems, indexed by i. The force (affector or cause) upon any subsystem is given by a vector $\mathbf{F}_i$. The constitutive properties of any subsystem are given by a vector $\mathbf{a}^i$. It is postulated that the dynamical response of the system to a set of imposed forces $\{\mathbf{F}_i\}$ is given by a dyadic $\underset{\sim}{\mathbf{R}} \equiv \mathbf{a}^i\mathbf{F}_i$ (Einstein summation) called the response tensor. There are many ways to describe the dynamics in this manner, and it is postulated that $\underset{\sim}{\mathbf{R}}$ is invariant under such transformations. This is analogous to the invariance of a radius vector $\mathbf{R} = \mathbf{e}^i x_i$ under co-ordinate transformations. Using the techniques of metric geometry, it is shown that these simple postulates lead to a phenomenological dynamics with a structure similar to irreversible thermodynamics (a special case of a phenomenological calculus).

In particular, it is shown that if $\{\mathbf{a}_i\}$ and $\{\mathbf{J}^i\}$ belong to the space dual to $\{\mathbf{a}^i\}$ and $\{\mathbf{F}_i\}$, then $\mathbf{J}^i = L^{ij}\mathbf{F}_j$, where $L^{ij} = \mathbf{a}^i \cdot \mathbf{a}^j$ are elements of a metric tensor. This gives a canonical relationship between forces (or causes) and resultant fluxes (or effects), denoted $\mathbf{J}^i$. By definition, $L^{ij} = L^{ji}$. Furthermore, there is a principle of directionality: $|\underset{\sim}{\mathbf{R}}|^2 \equiv \underset{\sim}{\mathbf{R}} : \underset{\sim}{\mathbf{R}} = L^{ij}\mathbf{F}_i \cdot \mathbf{F}_j \geq 0$. In the special case of irreversible thermodynamics, this is simply the Second Law: $|\underset{\sim}{\mathbf{R}}|^2 = \delta \geq 0$, where δ is the dissipation function. What is remarkable, is that this positive–definite condition results from the postulates defining a response tensor and is not assumed as a physical law. The paper ends with a discussion applying the phenomenological calculus to problems of aging.

1. Introduction

Biological systems are in general far too complex to be analysed by a reduction to their underlying dynamics. The specification of such detailed dynamics is, to say the least, formidable, and the solution often unimaginable. However, this is not the only way to address complex systems and,

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in fact, is not necessarily the most informative. The mathematical investigation of biological systems has produced a wealth of alternative methods: for example, the set-theoretic approach of Rashevsky (1960), Rosen's (1978) use of category theory, the mathematical ecology of May (1974), the dissipative structures of Nicolis & Prigogine (1977), the catastrophe theory of Thom (1975), the net-work thermodynamics of Oster, Perelson & Katchalsky (1973), and the synergetics of Haken (1978).

In this paper we will develop a calculus which in lieu of a comprehensive dynamics relates in a phenomenological manner the forces operating upon a complex system to the resultant motions—or in the biological context, effects are related to generalized causes. The mathematical connection between forces and fluxes (or causes and effects) is not directly established but rather is given as the consequence of postulating that the complex interactions of the system with its environment can be described in terms of a "response" tensor which is a simple function of the imposed forces and a set of constitutive parameters for the system. Under the additional assumption that this response tensor is an invariant as regards system description, a phenomenological calculus relating forces and fluxes in a canonical manner is derived.

This calculus has a metrical structure, and the squared norm on the space spanned by the response tensor gives a principle of directionality. For physical systems, this principle of directionality is simply the Second Law of Thermodynamics. In the biological context, this principle can be interpreted as an indicator of the aging that is universal to all complex biological systems. This principle of directionality is remarkable because it is inherent in the formulation of the response tensor: that is, it is not brought, as it were, from outside as a physical law. Furthermore, the existence of a metric associated with a system dynamics allows a precise measure of dynamical similitudes. With the norm, one can measure the "distance" between the response tensors of two different systems or between the responses of a given system to two different sets of environmental forces.

2. The Response Tensor and Description Space

The concept of the response tensor was originally presented (Richardson, 1980) in the context of irreversible thermodynamics. This still seems the best way to motivate the discussion, as it appeals strongly to physical intuition and offers a familiar notation. Later it will be shown that the concept is general and is in no way restricted to thermodynamic systems.

The primary goal of irreversible thermodynamics is the formulation of linear dynamical equations for the fluxes, $\mathbf{J}^i$, of a system of molecules and ions, indexed according to species by i. It is posited that if the dissipation function of the system is derived in the form $\delta = \mathbf{F}_i . \mathbf{J}^i$ (Einstein summation notation), then the fluxes are given phenomenologically as a linear function of the conjugate set of forces: that is,

$$\mathbf{J}^i = L^{ij}\mathbf{F}_j. \tag{1}$$

Moreover, extrapolating from Onsager's theory of fluctuations, it is assumed that the matrix of phenomenological coefficients is symmetric: that is, $L^{ij} = L^{ji}$. The Second Law of Thermodynamics requires that the dissipation function be positive definite: that is, $\delta \geq 0$.

In Richardson (1980), a metric algebra based upon the dissipation function associated with a system was introduced. The analogy between the norm of a radius vector in Euclidean space and the norm of a radius (response) tensor in a so-called description space was developed, thereby establishing a means for investigating the metric structure inherent in the dynamics of systems which age. The derivation of the response tensor, $\underset{\sim}{\mathbf{R}}$, was motivated by the resemblance of the dissipation function, $\delta = L^{ij}\mathbf{F}_i . \mathbf{F}_j$, to the squared norm of a radius vector in skew rectilinear coordinates, $|\mathbf{R}|^2 = g^{ij}x_i x_j$, where g^{ij} is an element of the fundamental metric tensor. It was demonstrated that, indeed, $\delta = |\underset{\sim}{\mathbf{R}}|^2$ for a response tensor defined by the dyadic

$$\underset{\sim}{\mathbf{R}} \equiv \mathbf{a}^i\mathbf{F}_i. \tag{2}$$

The set of vectors $\{\mathbf{a}^i\}$ are constitutive parameters characteristic of a given system. In the definition (2), the $\mathbf{a}^i$ are analogous to the fixed set of basis vectors for a given skew rectilinear co-ordinate system in Euclidean space. The set of vectors $\mathbf{F}_i$ comprise the possible forces which might bear upon the system. They range freely and are analogous to the components, x_i, of any possible radius vector in the above-mentioned rectilinear co-ordinate system.

It was shown that the response tensors formed a metric space with a squared norm given by the double-dot product $|\underset{\sim}{\mathbf{R}}|^2 \equiv \underset{\sim}{\mathbf{R}} : \underset{\sim}{\mathbf{R}}$ and that $|\underset{\sim}{\mathbf{R}}|^2 = L^{ij}\mathbf{F}_i . \mathbf{F}_j$. The space spanned by $\underset{\sim}{\mathbf{R}}$ was called the description space. However, in that first paper on the response tensor, the crucial condition $\underset{\sim}{\mathbf{R}}^2 \geq 0$ was assumed *a priori* because the Second Law dictates that $\delta \geq 0$. Thus the positive definiteness of the norm was given by physical reasoning. In the present paper, it will be demonstrated that $|\underset{\sim}{\mathbf{R}}|^2 \geq 0$ is actually a mathematical consequence of the definition of description space.

3. The Metrical Structure of Description Space

Before proceeding to a formal mathematical examination of the response tensor and its implications for the analysis of dynamical systems, it will be instructive to make explicit the basic assumptions more or less implicit in Richardson (1980). The phenomenological calculus arising from the metrical structure of description space is based upon three postulates:

Postulate 1. The specification of the forces, $\{\mathbf{F}_i\}$, acting upon a system and the set of the constitutive parameters, $\{\mathbf{a}^i\}$, conjugate to those forces is sufficient to determine a phenomenological description of the system dynamics.

Postulate 2. The system dynamics is characterized phenomenologically by the response tensor $\underline{\mathbf{R}} \equiv \mathbf{a}^i\mathbf{F}_i$.

Definition. The space spanned by $\underline{\mathbf{R}}$ is called description space.

Postulate 3. The response tensor is invariant under co-ordinate transformations in description space.

That the familiar equations of irreversible thermodynamics are a consequence of these postulates is demonstrated schematically in Fig. 1. On the left hand side of the figure, we see the specification of the components $\mathbf{F}_i$ and the co-ordinate vectors $\mathbf{a}^i$. Within this co-ordinate system, the response tensor which characterizes the dynamics of the system is simply $\underline{\mathbf{R}} = \mathbf{a}^i\mathbf{F}_i$. However, there are other co-ordinates which describe the system and which, by Postulate 3, give the same response tensor. Of particular

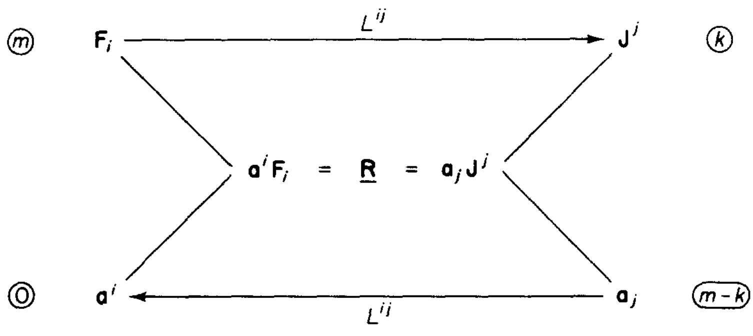

FIGURE 1.

interest are the co-ordinates $\{\mathbf{a}_i\}$ in the dual space of $\{\mathbf{a}^i\}$. The components dual to $\{\mathbf{F}_i\}$ (denoted $\mathbf{J}^i$) are defined by the projection of $\underline{\mathbf{R}}$ upon the co-ordinate vector $\mathbf{a}^i$: that is

$$\begin{aligned} \mathbf{J}^i &\equiv \mathbf{a}^i . \underline{\mathbf{R}} \\ &= (\mathbf{a}^i . \mathbf{a}^j)\mathbf{F}_j \\ &= L^{ij}\mathbf{F}_j. \end{aligned} \tag{3}$$

By definition $L^{ij} \equiv \mathbf{a}^i . \mathbf{a}^j$, and by the symmetry of the dot product, $L^{ij} = L^{ji}$. Thus one finds the elements, L^{ij}, of the fundamental metric tensor for description space. The norm, the triangle inequality, and the other relationships given in the preceding discussion were then calculated in a straightforward manner in Richardson (1980).

This original presentation was rather intuitive, proceeded mainly by the analogy between the response tensor and a radius vector, and established the condition $|\underline{\mathbf{R}}| \geq 0$ by bringing in a physical law from outside the mathematical formalism of the response tensor. We shall now re-examine the concept of the response tensor in more precise mathematical terms. It will be demonstrated that the three postulates are themselves a sufficient foundation for deriving a phenomenological calculus for complex dynamical systems. This calculus has a metrical structure and a principle of directionality. Moreover, as will be shown, the formalism can be extended to description spaces wherein the L^{ij} are not constants—to what one might call Riemannian description spaces.

4. The Space of Dyadics

We shall begin by looking at dyadics in more detail. Let V be the vector space $\mathbb{R}^n$ and let it be equipped with the standard inner (dot) product. Let $\{\mathbf{e}_i\} = \{\mathbf{e}_1 = (1, 0, \ldots, 0), \mathbf{e}_2 = (0, 1, 0, \ldots, 0), \ldots, \mathbf{e}_n = (0, \ldots, 0, 1)\}$ be the standard basis for $\mathbb{R}^n$. The formalism can easily be generalized to any finite-dimensional inner product space and an orthonormal basis. However, the Euclidean space $\mathbb{R}^n$ is sufficient for our purpose. Any contravariant vector $\mathbf{F} \in V$ can be expressed uniquely as $\mathbf{F} = x^i\mathbf{e}_i = (x^1, x^2, \ldots, x^n)$. Let V^* be the dual space of V and let $\{\mathbf{e}^i\}$ be the dual basis of $\{\mathbf{e}_i\}$. (Since $\{\mathbf{e}_i\}$ is orthonormal we actually have $\mathbf{e}^i = \mathbf{e}_i$, but we shall use $\mathbf{e}^i$ to keep the ideas straight.) Then any covariant vector $\mathbf{a} \in V^*$ can be expressed uniquely as $\mathbf{a} = y_i\mathbf{e}^i = (y_1, y_2, \ldots, y_n)$.

Definition 1: Let $\mathbf{F} \in V$ and $\mathbf{a} \in V^*$. Then the *dyad* $\underline{\mathbf{R}} = \mathbf{aF}$ is a bilinear mapping from $V^* \times V$ to $\mathbb{R}$ defined by $\underline{\mathbf{R}}(\mathbf{a}', \mathbf{F}') = (\mathbf{aF}) : (\mathbf{a}'\mathbf{F}') = (\mathbf{a} . \mathbf{a}')(\mathbf{F} . \mathbf{F}')$, where the second equality is, incidentally, the definition of the double dot product of dyads.

In terms of components, if $\mathbf{F}=x^i\mathbf{e}_i$, $\mathbf{a}=y_i\mathbf{e}^i$, $F'=x^{i'}\mathbf{e}_i$, $\mathbf{a}'=y'_i\mathbf{e}^i$, then $\underline{\mathbf{R}}(\mathbf{a}',\mathbf{F}')=(y_iy'_i)(x^jx^{j'})\in\mathbb{R}$. In particular, we define the components of the dyad $\underline{\mathbf{R}}$ to be $R^j_i=\underline{\mathbf{R}}(\mathbf{e}^i,\mathbf{e}_j)=y_ix^j\in\mathbb{R}$ for $i,j=1,\ldots,n$. Thus we can identify $\underline{\mathbf{R}}$ with an $n\times n$ real matrix

$$\underline{\mathbf{R}}=(R^j_i)=\begin{pmatrix} y_1x^1 & y_1x^2 & \ldots & y_1x^n \\ y_2x^1 & \cdot & & \cdot \\ \vdots & & \cdot & \cdot \\ & & \cdot & \cdot \\ y_nx^1 & \ldots & & y_nx^n \end{pmatrix} \tag{4}$$

and

$$\underline{\mathbf{R}}(\mathbf{a}',\mathbf{F}')=(y'_1,\ldots,y'_n)(R^j_i)\begin{pmatrix} x^{1'} \\ \vdots \\ x^{n'} \end{pmatrix}. \tag{5}$$

In the language of tensor theory, a bilinear mapping from $V^*\times V$ to $\mathbb{R}$ is a tensor of type $(1,1)$ over V. The n^{r+s} dimensional vector space of all tensors of type (r,s) over V is denoted by $T^r_s(V)$ or

$$\underbrace{V\otimes\ldots\otimes V}_{r}\otimes\underbrace{V^*\otimes\ldots\otimes V^*}_{s};$$

so we have the dyad $\underline{\mathbf{R}}\in T^1_1(V)=V\otimes V^*$.

Definition 2. Let $r\in\mathbb{R}$. Then $r\underline{\mathbf{R}}$ is defined as the bilinear mapping $V^*\times V\to\mathbb{R}$ by $(r\underline{\mathbf{R}})(\mathbf{a}',\mathbf{F}')=r(\underline{\mathbf{R}}(\mathbf{a}',\mathbf{F}'))$.

Note that $r\underline{\mathbf{R}}=r(\mathbf{aF})=(r\mathbf{a})\mathbf{F}=\mathbf{a}(r\mathbf{F})$ so $r\underline{\mathbf{R}}$ is a dyad. Also, $(rR)^j_i=r(R^j_i)$.

Definition 3. If $\underline{\mathbf{R}}$ and $\underline{\mathbf{S}}$ are dyads, then $\underline{\mathbf{R}}+\underline{\mathbf{S}}$ is defined as the bilinear mapping $V^*\times V\to\mathbb{R}$ by $(\underline{\mathbf{R}}+\underline{\mathbf{S}})(\mathbf{a}',\mathbf{F}')=\underline{\mathbf{R}}(\mathbf{a}',\mathbf{F}')+\underline{\mathbf{S}}(\mathbf{a}',\mathbf{F}')$.

Note that $(R+S)^j_i=(\underline{\mathbf{R}}+\underline{\mathbf{S}})(\mathbf{e}^i,\mathbf{e}_j)=R^j_i+S^j_i$. But in general $\underline{\mathbf{R}}+\underline{\mathbf{S}}$ cannot be expressed as $\mathbf{aF}$ for some $\mathbf{a}\in V^*$ and $\mathbf{F}\in V$. So the finite sums of dyads are not necessarily dyads although they are still in $T^1_1(V)$.

Definition 4. A finite sum of dyads is called a *dyadic*, and it is a bilinear mapping $V^*\times V\to\mathbb{R}$.

It is clear that we have the following "distributive laws":

$$\begin{aligned} \mathbf{a}(\mathbf{F}_1+\mathbf{F}_2)&=\mathbf{aF}_1+\mathbf{aF}_2 \\ (\mathbf{a}^1+\mathbf{a}^2)\mathbf{F}&=\mathbf{a}^1\mathbf{F}+\mathbf{a}^2\mathbf{F}. \end{aligned} \tag{6}$$

Let S be the set of all dyadics $\{\underset{\sim}{\mathbf{R}}=\sum_{i=1}^{m}\mathbf{a}^i\mathbf{F}_i: m \text{ finite}, \mathbf{a}^i\in V^*, \mathbf{F}_i\in V\}$. Then S is the linear subspace of $T_1^1(V)$ generated by the dyads. In fact, we have the following

Theorem 1. $S=T_1^1(V)=V\otimes V^*$

Proof. For each $i, j=1,\ldots,n$,

$$\underset{\sim}{\mathbf{E}}_j^i=\mathbf{e}^i\mathbf{e}_j=i\begin{pmatrix} 0 & \cdots & \overset{j}{0} & \cdots & 0\\ \vdots & & \vdots & & \vdots\\ 0 & \cdots & 1 & \cdots & 0\\ \vdots & & \vdots & & \vdots\\ 0 & \cdots & 0 & \cdots & 0\end{pmatrix}=(\delta_j^i) \tag{7}$$

is in S. But $\{\underset{\sim}{\mathbf{E}}_j^i\}$ is a basis for $T_1^1(V)$. Hence $S=T_1^1(V)$ and so the space of dyadics is a vector space of dimension n^2 over $\mathbb{R}$ □

Let $\underset{\sim}{\mathbf{R}}$ be a dyadic. Then $\underset{\sim}{\mathbf{R}}=R_i^j\underset{\sim}{\mathbf{E}}_j^i=R_i^j\mathbf{e}^i\mathbf{e}_j=\mathbf{e}^i(R_i^j\mathbf{e}_j)=\mathbf{e}^i\mathbf{R}_i$ where $\mathbf{R}_i=R_i^j\mathbf{e}_j\in V$. So we see that every dyadic can be expressed as a sum of (at most) n dyads. Also, $\underset{\sim}{\mathbf{R}}=\underset{\sim}{\mathbf{0}}$ (i.e. the bilinear function from $V^*\times V$ to $\mathbb{R}$ which maps everything to the number 0) iff all $R_i^j=0$ iff all $\mathbf{R}_i=0$. This argument can easily be generalized to an arbitrary basis for V^* (and of course the dual statement for V also holds) and we have the

Theorem 2. Let $\mathbf{a}^i$ be a basis for V^*. Then every dyadic $\underset{\sim}{\mathbf{R}}$ can be written as $\underset{\sim}{\mathbf{R}}=\mathbf{a}^i\mathbf{F}_i$ (at most n terms) for an appropriately chosen set of vectors $\mathbf{F}_i\in V$. Further, $\underset{\sim}{\mathbf{R}}=\underset{\sim}{\mathbf{0}}$ iff all $\mathbf{F}_i=\mathbf{0}$, and hence the representation $\underset{\sim}{\mathbf{R}}=\mathbf{a}^i\mathbf{F}_i$ is unique. (I.e. if $\underset{\sim}{\mathbf{R}}=\mathbf{a}^i\mathbf{F}_i=\mathbf{a}^i\mathbf{F}'_i$, then $\mathbf{F}_i=\mathbf{F}'_i$ for all i.) □

Corollary. For a fixed basis $\mathbf{a}^i$ of V^*, $\{\underset{\sim}{\mathbf{R}}=\mathbf{a}^i\mathbf{F}_i: \mathbf{F}_i\in V\}=T_1^1(V)=V\otimes V^*$. □

Definition 5. Let $\underset{\sim}{\mathbf{R}}=\mathbf{e}^i\mathbf{R}_i$ and $\underset{\sim}{\mathbf{S}}=\mathbf{e}^i\mathbf{S}_i$ be dyadics, then their *double dot product* is defined as the real number $\underset{\sim}{\mathbf{R}}:\underset{\sim}{\mathbf{S}}=(\mathbf{e}^i.\mathbf{e}^j)(\mathbf{R}_i.\mathbf{S}_j)=\mathbf{R}_i.\mathbf{S}_i$ (because $\{\mathbf{e}^i\}$ is orthonormal).

Theorem 3. Let $\underset{\sim}{\mathbf{R}}=\sum_{\lambda=1}^{l}\mathbf{a}^\lambda\mathbf{F}_\lambda$ and $\underset{\sim}{\mathbf{S}}=\sum_{\mu=1}^{m}\mathbf{b}^\mu\mathbf{G}_\mu$ be two arbitrary representations of the dyadics $\underset{\sim}{\mathbf{R}}$ and $\underset{\sim}{\mathbf{S}}$, then

$$\underset{\sim}{\mathbf{R}}:\underset{\sim}{\mathbf{S}}=\sum_{\mu=1}^{m}\sum_{\lambda=1}^{l}(\mathbf{a}^\lambda.\mathbf{b}^\mu)(\mathbf{F}_\lambda.\mathbf{G}_\mu).$$

Proof. Formal manipulation—reduce everything to linear combinations of the basis $\{\mathbf{e}_i\}$ and $\{\mathbf{e}^i\}$. □

So Theorem 3 says that the double dot product is independent of the representation and is in particular independent of the basis, one simply expands formally according to the distributive law (: distributive over +).

Theorem 4. For any dyadic $\underline{\mathbf{R}}$, $|\underline{\mathbf{R}}|^2 = \underline{\mathbf{R}} : \underline{\mathbf{R}} \geq 0$, and $|\underline{\mathbf{R}}|^2 = 0$ iff $\underline{\mathbf{R}} = \underline{\mathbf{0}}$.

Proof. $|\underline{\mathbf{R}}|^2 = \underline{\mathbf{R}} : \underline{\mathbf{R}} = \sum_{i=1}^{m} \mathbf{R}_i . \mathbf{R}_i \geq 0$ and $= 0$ iff all $\mathbf{R}_i = \mathbf{0}$. □

The double dot product as a mapping from $T_1^1(V) \times T_1^1(V)$ to $\mathbb{R}$ is clearly a symmetric bilinear form. Theorem 4 says it is positive definite. This gives

Theorem 5: $(T_1^1(V), :)$ is an inner product space. □

5. The Description Space

Let us now rephrase the three postulates of section 3 in the formalism we have just developed.

Postulate 1. A given system is characterized by a set of vectors $\mathbf{a}^i$ ($i = 1, 2, \ldots, m$) in (the dual space of) $\mathbb{R}^n$, and this set depends upon the physical constitution of the system. As far as describing the dynamic response of the system to the imposition of a set of forces (or more generally, *causes*) $\mathbf{F}^i$ in $\mathbb{R}^n$, they form a complete set of constitutive parameters. The index i denotes subsystems (monads, elements, molecular species, organ systems, etc.) of the system.

Postulate 2. The system dynamics are characterized phenomenologically by the dyadic response tensor $\underline{\mathbf{R}} = \mathbf{a}^i \mathbf{F}_i$.

Postulate 3. The space spanned by $\underline{\mathbf{R}}$—i.e. for fixed covariant vectors $\mathbf{a}^1, \ldots, \mathbf{a}^m$ in $V^* \cong \mathbb{R}^n$, the set $D = \{\underline{\mathbf{R}} = \mathbf{a}^i \mathbf{F}_i : \mathbf{F}_i \in V = \mathbb{R}^n\}$—is called the description space, and $\underline{\mathbf{R}}$ is invariant under co-ordinate transformations in D.

Thus, in our formalism of dyadics as elements of the tensor space $T_1^1(V)$, the description space becomes a linear subspace of $T_1^1(V)$. Also, it is clear that if the dimension (over $\mathbb{R}$) of the linear subspace of V^* spanned by $\{\mathbf{a}^i\}$ is k ($\therefore k \leq n$), then the dimension of D (over $\mathbb{R}$) is kn ($\leq n^2 = \dim T_1^1(V)$). Note that $\{\mathbf{a}^i\}$ is not required to be a basis of V^*, and in fact it is not even assumed to be a linearly independent set. Thus, although it is similar to a fixed set of basis vectors in $\mathbb{R}^n$, to avoid confusion we shall refer to $\{\mathbf{a}^i\}$ as the set of *co-ordinate vectors* and not basis vectors.

We now have

Theorem 6. $(D, :)$ is an inner product space and so in particular for all $\underset{\sim}{\mathbf{R}} \in D$, $|\underset{\sim}{\mathbf{R}}|^2 = \underset{\sim}{\mathbf{R}} : \underset{\sim}{\mathbf{R}} \geq 0$ and $|\underset{\sim}{\mathbf{R}}|^2 = 0$ iff $\underset{\sim}{\mathbf{R}} = \underset{\sim}{0}$. □

Note very carefully, however, that if $\underset{\sim}{\mathbf{R}} = \mathbf{a}^i\mathbf{F}_i \in D$ is such that $|\underset{\sim}{\mathbf{R}}|^2 = 0$, we have only $\underset{\sim}{\mathbf{R}} = \underset{\sim}{0}$ and not necessarily all $\mathbf{F}_i = \mathbf{0}$. In fact $|\mathbf{R}|^2 = 0 \Leftrightarrow$ all $\mathbf{F}_i = \mathbf{0}$ if and only if $\{\mathbf{a}^i\}$ is linearly independent in V^*.

6. The Phenomenological Calculus

In the preceding exposition on the mathematical character of the response tensor, we have, in effect, established a phenomenological calculus having the same structure as irreversible thermodynamics. The applicability of this calculus is, however, far more general, being based solely upon three abstract postulates without recourse to physical principles. With the notation and results developed above, such a general phenomenology can be quickly derived.

The components, $\{\mathbf{F}_i\}$ need not be restricted to physical forces: for example, those of transport theory, which are given as the negative gradient of the electrochemical potential of molecular species i. They may be considered general affectors in the system dynamics, arising from interactions between the various subsystems (indexed by i) or as affectors upon subsystems which are generated outside the system. To make quite clear that the $\{\mathbf{F}_i\}$ need not be physical forces, we shall now call them "causes". In medicine, an example of such a set of cause vectors would be the epidemiologist's set of risk factors for the causes of aging, with the index i denoting the various organs upon which measurements of aging processes are made.

As before, the response of the system to an imposed set of causes is given by the response tensor. In dynamical systems, causes give rise to "effects", and we have at hand a formal means for calculating a canonical set of effects. The effects are simply the set of components in the dual space (for convenience, the notation $\mathbf{J}^i$ for this dual set will be retained). Let us put this more precisely.

Since a dyadic $\underset{\sim}{\mathbf{R}} = \mathbf{a}^i\mathbf{F}_i$ is defined as a bilinear mapping from $V^* \times V$ to $\mathbb{R}$ via $\underset{\sim}{\mathbf{R}}(\mathbf{a}, \mathbf{F}) = \underset{\sim}{\mathbf{R}} : (\mathbf{aF}) = (\mathbf{a}^i . a)(\mathbf{F}_i . \mathbf{F})$ (sum over i), it follows that if we fix

$\mathbf{a} \in V^*$, then $\underline{\mathbf{R}}(\mathbf{a}, .): V \to \mathbb{R}$ is a linear map, i.e. (by definition) $\underline{\mathbf{R}}(\mathbf{a}, .) = (\mathbf{a}^i . \mathbf{a})\mathbf{F}_i \in V^*$. In particular, we have the

Definition. Given a set of causes, $\{\mathbf{F}_i\}$, let $\underline{\mathbf{R}} = \mathbf{a}^i \mathbf{F}_i$ be a response tensor in the description space D. Then for $j = 1, \ldots, m$, the effects are

$$\mathbf{J}^j = \underline{\mathbf{R}}(\mathbf{a}^j, .) = (\mathbf{a}^i . \mathbf{a}^j)\mathbf{F}_i \in V^*. \tag{8}$$

Now $\mathbf{J}^j = (\mathbf{a}^i . \mathbf{a}^j)\mathbf{F}_i$ is a relation between "causes" and "effects". Again borrowing language from irreversible thermodynamics, we define "phenomenological coefficients" as

$$L^{ij} = \mathbf{a}^i . \mathbf{a}^j \tag{9}$$

and thus

$$\mathbf{J}^j = L^{ij}\mathbf{F}_i. \tag{10}$$

Note that the Onsager reciprocal relation $L^{ij} = L^{ji}$ is now a consequence of the definition, because trivially $\mathbf{a}^i . \mathbf{a}^j = \mathbf{a}^j . \mathbf{a}^i$.

Furthermore, the squared-norm of the response tensor is

$$|\underline{\mathbf{R}}|^2 = \underline{\mathbf{R}} : \underline{\mathbf{R}} = (\mathbf{a}^i . \mathbf{a}^j)(\mathbf{F}_i . \mathbf{F}_j) = L^{ij}\mathbf{F}_i . \mathbf{F}_j = \mathbf{J}^j . \mathbf{F}_j. \tag{11}$$

But $\mathbf{J}^j . \mathbf{F}_j$ in irreversible thermodynamics is precisely the definition of the dissipation function δ; i.e. we have

$$|\underline{\mathbf{R}}|^2 = \mathbf{J}^j . \mathbf{F}_j = \delta \tag{12}$$

and it follows from the positive definiteness of the squared-norm that $\delta \geq 0$, hence the Second Law of Thermodynamics is also a consequence of our formalism.

The condition $|\underline{\mathbf{R}}|^2 \geq 0$ is a general condition which holds for all cause-and-effect phenomenologies, not only for irreversible thermodynamics. Rather than burden it with physical connations by calling it a generalized Second Law, one might give it the more representative cognomen of "the principle of directionality". In certain situations, the squared norm may provide a measure of the unidirectional aging of a system. Or, just as $\delta > 0$ characterizes a real physical system and $\delta = 0$ characterizes an ideal physical system, the condition $|\underline{\mathbf{R}}|^2 > 0$ says, in effect, that for a system to respond in a "real" way to its environment it must pay a price. Be that as it may, the condition $|\underline{\mathbf{R}}|^2 \geq 0$ prompts the definition

$$|\underline{\mathbf{R}}|^2 \equiv \left(\frac{d\tau}{dt}\right)^2 \tag{13}$$

for systems where the dynamics are parameterized by a standard time kept by an ideal harmonic oscillator: see Richardson & Rosen (1979). This definition provides a proper time, τ, which can serve as a measure of aging and also provides the mathematical form which will allow the examination of Riemannian description spaces to be given in section 8.

7. The Dual Representation of a Response Tensor

The Oxford dictionary defines "cause" as "that which produces an effect". Intuitively one thinks of the relation between causes and effects in such a way that if the causes are somehow "given", then the effects can, at least in principle, be derived. When the effects are known, however, it is usually very difficult, if not impossible, to determine the causes uniquely. An example of this is given by medical diagnosis, in which the effects (symptoms) are observables, hence known, and one attempts to find the causes from this set of observable effects. One often feels that "more information" is required if the causes (of the diseases, in this case) are to be determined.

The fact that effects are derivable from causes is reflected in the equation

$$\mathbf{J}^j = L^{ij}\mathbf{F}_i. \tag{14}$$

Let us now investigate why we cannot in general obtain $\{\mathbf{F}_i\}$ even if all the values of $\{\mathbf{J}^j\}$ are known.

In the Euclidean space $V=\mathbb{R}^n$ with basis $\{\mathbf{e}_i\}$, a radius vector $\mathbf{R}=x^i\mathbf{e}_i$ has a representation in the dual space $V^*\cong R^n$ as $\mathbf{R}=x_j\mathbf{e}^j$, where $\{\mathbf{e}^j\}$ is the dual basis in V^* to $\{\mathbf{e}_i\}$ in V. The metric tensor with components $g_{ij}=\mathbf{e}_i\,.\,\mathbf{e}_j$ is invertible and its inverse has components $g^{ij}=\mathbf{e}^i\,.\,\mathbf{e}^j$. The various vectors and components are related by

$$\begin{aligned} \mathbf{e}^j &= g^{ij}\mathbf{e}_i, & \mathbf{e}_i &= g_{ij}\mathbf{e}^j, \\ x_j &= g_{ij}x^i, & x^i &= g^{ij}x_j. \end{aligned} \tag{15}$$

So we have the representation diagram shown in Fig. 2.

Proceeding analogously, suppose we now want to find a dual representation of a response tensor $\underset{\sim}{\mathbf{R}}=\mathbf{a}^i\mathbf{F}_i$ in the description space D. Since the phenomenological equations

$$\mathbf{J}^j = L^{ij}\mathbf{F}_i \tag{16}$$

resemble

$$x^j = g^{ij}x_i, \tag{17}$$

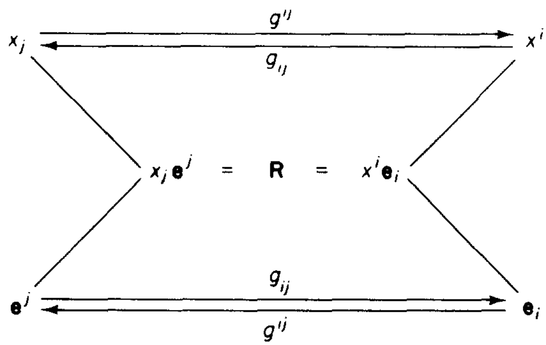

FIGURE 2.

and the phenomenological coefficients

$$L^{ij} = \mathbf{a}^i . \mathbf{a}^j \tag{18}$$

resemble

$$g^{ij} = \mathbf{e}^i . \mathbf{e}^j, \tag{19}$$

it is natural to look for a dual representation of $\underset{\sim}{\mathbf{R}}$ in the form

$$\underset{\sim}{\mathbf{R}} = \mathbf{a}_j \mathbf{J}^j, \tag{20}$$

where $\mathbf{a}_1, \ldots, \mathbf{a}_m$ are unknown vectors in $V = \mathbb{R}^n$ to be found. Substituting equation (16) into equation (20) we obtain

$$\underset{\sim}{\mathbf{R}} = \mathbf{a}^i \mathbf{F}_i = \mathbf{a}_j L^{ij} \mathbf{F}_i. \tag{21}$$

Thus

$$(\mathbf{a}^i - \mathbf{a}_j L^{ij}) \mathbf{F}_i = \underset{\sim}{\mathbf{0}} \tag{22}$$

for all choices of $\mathbf{F}_1, \ldots, \mathbf{F}_m$ in V, and hence

$$\mathbf{a}^i - \mathbf{a}_j L^{ij} = \mathbf{0} \tag{23}$$

in V^*; i.e.

$$L^{ij} \mathbf{a}_j = \mathbf{a}^i. \tag{24}$$

So, if the $m \times m$ matrix (L^{ij}) is invertible with inverse (L_{ij}), then the unique solution to equation (24) is

$$\mathbf{a}_j = L_{ij} \mathbf{a}^i. \tag{25}$$

Indeed this is the case for the metric tensor (g^{ij}). But our matrix (L^{ij}), is in general *not* invertible, it being the so-called Gram matrix of the vectors

$\{\mathbf{a}^i\}$ and being only positive *semi*-definite. (L^{ij}) has rank k (= the dimension of the subspace of V^* spanned by $\{\mathbf{a}^i\}$, hence $k \le m$ and n), and so we have $(m-k)$ degrees of freedom in picking the solution $\mathbf{a}_j$ to equation (24) (i.e. we can pick $m-k$ of the m vectors arbitrarily and the rest would then be determined).

So, in the description space D with fixed constitutive parameters $\{\mathbf{a}^i\}$, we have the representation indicated in Fig. 1 (where the circled numbers are the degrees of freedom in picking the corresponding set of vectors—note the balance of degrees of freedom on both sides: $m+0 = k+(m-k)$).

The major difference between Figs 1 and 2 lies in the fact that the arrows in Fig. 2 are reversible whereas in Fig. 1 they are not. This means that when we pass from the causes $\mathbf{F}_i$ to the effects $\mathbf{J}^i$, we have lost some information—the causes determine the effects uniquely via equation (16) but not vice versa. And with only the effects $\mathbf{J}^i$, we have to know more about the "dual constitutive parameters" $\mathbf{a}_j$ in order to determine the response $\underline{\mathbf{R}}$ and hence find the causes $\mathbf{F}_i$ uniquely. Interpreted within the context of our example of medical diagnosis, this says that if the causes (of a disease) are to be firmly decided on, one needs to know not only all the symptoms but some of the constitution of the system as well.

8. Riemannian Description Spaces and Aging

Although no mention has been made of any possible functional dependence of the vectors $\{\mathbf{a}^i\}$ upon the forces $\{\mathbf{F}_i\}$, one must not conclude that the $\{\mathbf{a}^i\}$ are necessarily constants. That is, one must not conclude that all description spaces are Euclidean, with elements, $L^{ij} = \mathbf{a}^i . \mathbf{a}^j$, of the metric tensor independent of the components, $\{\mathbf{F}_i\}$, in D-space (analogous to the g^{ij} being independent of the components $\{x_i\}$). In fact, none of the proofs given in the preceding sections has assumed that the $(\mathbf{a}^i\}$ are constants. The results are valid in general. The possibility of Riemannian description spaces greatly increases the scope of application of the phenomenological calculus, giving in particular some interesting insights into irreversible thermodynamics and into aging processes.

One of the maxims of classical irreversible thermodynamics is that the phenomenological coefficients, L^{ij}, are independent of the forces and fluxes. While this seems physically plausible, it is a little unsettling mathematically. The coefficients are scalars, and any dependence upon the vector forces and fluxes would be by various dot-products. One then wonders about the underlying physical meaning which could be ascribed to such a dependence. From the viewpoint of the proposed phenomenological calculus, this maxim of independence is seen as a constraint upon the geometric structure of the description space underlying classical irreversible thermodynamics. The condition that the constitutive vectors $\{\mathbf{a}^i\}$ are independent of forces and fluxes is simply a restriction to a Euclidean D-space.

However, the metric geometry associated with the response tensor is not itself restricted to a Euclidean description space. Therefore, an interesting possibility appears. If, indeed, irreversible thermodynamics is based upon the concept of the response tensor (they are mathematically indistinguishable) there is no prohibition against the dependence

$$\mathbf{a}^i = \mathbf{a}^i(\mathbf{F}_1, \mathbf{F}_2 \ldots \mathbf{F}_m). \tag{26}$$

Thus, through this vector equation, the elements L^{ij} become functions of the components $\{\mathbf{F}_i\}$, and the D-space becomes Riemannian. As before, $|\underline{\mathbf{R}}|^2 \equiv \delta \geq 0$ and the linear relationships $\mathbf{J}^i = L^{ij}\mathbf{F}_j$ still hold but only locally.

It has been noted earlier (Richardson & Rosen, 1979) that the formalism of irreversible thermodynamics leads to an "entropic" metric for time for certain classes of dynamical systems. Using dimensional analysis, they showed that the L^{ij} scaled the time-evolution of a system of coupled processes to a common time, denoted entropic time because of the relationship of the L^{ij} to the dissipation function (entropy production). The use of the term "metric of time" in that paper was suggestive, not precise, in that the techniques of dimensional analysis were not sufficient to discover the underlying metrical structure. Borrowing terminology, we have defined a proper time (13), which in some respects is similar to the entropic time of Richardson & Rosen (1979). It is, however, more general in application and is immediately based upon a metrical geometry—that of description spaces. Moreover, this proper time is not restricted to physical systems.

The condition $|\underline{\mathbf{R}}|^2 \geq 0$ assures that the proper time, τ, is a monotonically increasing function of the clock time, t, used to parameterize the system dynamics. For systems under the influence of constant forces, proper time is a linear function of clock time, with the elements, L^{ij}, of the metric tensor as scale factors: i.e.

$$\begin{aligned} d\tau &= \sqrt{L^{ij}\mathbf{F}_i.\mathbf{F}_j}\,dt \\ &= \sqrt{L^{ij}k_{ij}}\,dt \end{aligned} \tag{27}$$

where here $k_{ij} \equiv \mathbf{F}_i.\mathbf{F}_j$ and also L^{ij} are constants by virtue of $\mathbf{F}_i$ being assumed constant.

The principle of directionality, $|\underline{\mathbf{R}}|^2 \geq 0$, necessarily makes proper time an irreversible time. For systems wherein the forces (or generalized causes) are derivable from potential energy functions, the proper time is a direct measure of the production of entropy by the degradation of those potential energies. This could justify an assumption that proper time is a measure of the age of a complex dynamical system. This was suggested in Richardson (1980) where it was also proposed that the norm $|\mathbf{R}(a)-\mathbf{R}(b)|$ provided a measuring of the difference in aging between two systems a and b. There is no need to repeat that discussion here. It is, however, important to point out that this approach measures the age of the system dynamics, not of the system *per se*.

By Postulate 1, the system is characterized solely and sufficiently by the specification of the constitutive parameters $\{\mathbf{a}^i\}$. The aging of the system *per se* must be measurable by observation of changes in these $\{\mathbf{a}^i\}$. For example, collagen ages by cross-linking and this is observable macroscopically as changes in constitutive parameters such as Young's modulus. For a system which can be described by a phenomenological calculus framed in a Euclidean description space, the $\{\mathbf{a}^i\}$ are constants. The system perforce cannot age. Nevertheless, its dynamics ages with the proper time (13).

Consider now a system dynamics given in a Riemannian D-space. The constitutive parameters $\{\mathbf{a}^i\}$ have the dependence indicated in equation (26). If the forces change along the trajectory of the system dynamics, the $\{\mathbf{a}^i\}$ also change. One must be careful not to conclude that this represents system aging. There exists the possibility that the forces at any time, $\mathbf{F}_i(t)$, can be reset to their initial values, $\mathbf{F}_i(t_0)$. That would reset the values of the $\{\mathbf{a}^i\}$ to their initial values and all evidence of aging would vanish!

A piece of collagen which is continually stretched and flexed will age. The energy required for the increased cross-linking which is manifested as aging is the physical energy dissipated in the system. The proper time is a direct measure of the dissipation, and hence any changes in age-associated constitutive parameters should be functions of τ. In terms of our phenomenological calculus, a generalization of this would be to make the $\{\mathbf{a}^i\}$ be functions of proper time: that is,

$$\begin{aligned}\mathbf{a}^i &= \mathbf{a}^i[\mathbf{F}_1(t), \mathbf{F}_2(t) \ldots \mathbf{F}_m(t); \tau(t)]\\ &\equiv \mathbf{a}^i[\mathbf{F}(t); \tau(t)].\end{aligned} \tag{28}$$

Thus, the consideration of system aging as contrasted to the aging of system dynamics leads us to a Riemannian description space where the $\{\mathbf{a}^i\}$ are not only functions of the components, $\{\mathbf{F}_i\}$, but are also functions of the proper time (or path length). The defining equation (13) then becomes

$$\left(\frac{\mathrm{d}\tau}{\mathrm{d}t}\right)^2 = \{\mathbf{a}^i[\mathbf{F}(t); \tau(t)].\mathbf{a}^j[\mathbf{F}(t); \tau(t)]\}\{\mathbf{F}_i(t).\mathbf{F}_j(t)\}. \tag{29}$$

The exploration of this intriguing equation will be presented in a later paper. To formulate mathematical models for the dependence of the $\mathbf{a}^i$ (and hence the metric tensor) upon forces and proper time is to analyse directly the metrical structure underlying the system dynamics. In a modest way, this is similar to the situation in general relativity, where the dynamics of gravitation is essentially replaced by models for the effects of mass upon the curvature of spacetime.

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