

LETTER TO THE EDITOR

The Metric Structure of Irreversible Thermodynamics

A paper by Peusner (1986) came to our attention because of the notable similarity between his claims (of a Euclidean geometry of fluctuation-dissipation space) and what we established with mathematical rigour in our sequence of papers on the phenomenological calculus (see References), most of which were published in the *Journal of Theoretical Biology*.

Table 1 shows some of the direct correspondences between the formulation of our 1982 paper (Richardson *et al.*, 1982) and Peusner's 1986 paper. Note also that in Peusner there are inconsistencies and substantial confusion in the contra- and co-variant indices.

TABLE 1

Richardson & Louie	Peusner
\mathbf{a}^i	$\sqrt{g_{ii}} \mathbf{i}_i$
\mathbf{F}_i	α_i
$\mathbf{R} = \mathbf{a}^i \mathbf{F}_i$	$\boldsymbol{\xi} = \alpha_i \sqrt{g_{ii}} \mathbf{i}_i$ (sum over i)
$L^{ij} = \mathbf{a}^i \cdot \mathbf{a}^j$	g_{ij}
$\mathbf{J}^i = L^{ij} \mathbf{F}_j$	$X_i = g_{ij} \alpha_j$ (sum over j)
$\delta = \mathbf{R} ^2 = \mathbf{J}^i \cdot \mathbf{F}_i$	$2\Delta S = \boldsymbol{\xi} ^2 = 2\mathbf{X} \cdot \boldsymbol{\alpha}$

Note: in the Richardson-Louie formulation, the Einstein summation convention of summing over repeated upper and lower indices is used. In Peusner's formulation, the variances are confused.

We would like to present a representative sample of the many mathematical errors in Peusner's paper—some minor and others quite substantial.

- (1) In his equation (13), $X_i = -\partial\Delta S/\partial\alpha_i$, but in equation (14), the minus sign conveniently disappears. This confusion in sign has serious consequences. Since entropy is maximal at equilibrium, ΔS is negative definite, not "larger than zero" as stated by Peusner at the top of p. 135 and in equation (23).
- (2) In order that (g_{ij}) be a metric tensor consistent with Peusner's formulation, the *basis* would have to be

$$\{\sqrt{g_{11}} \mathbf{i}_1, \sqrt{g_{22}} \mathbf{i}_2\}$$

and not $\{\mathbf{i}_1, \mathbf{i}_2\}$ as (misleadingly) implied, nor $\{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2\}$ as claimed (after equations (17) and (18)).

- (3) At the bottom of p. 133, Peusner should have become alerted to his inconsistent usage of variances: note α_i in his earlier equations and $\boldsymbol{\alpha}^i$ in $\Delta S = \mathbf{X} \cdot \boldsymbol{\alpha}$.
- (4) In Section 4, Peusner confuses components with basis vectors. He appears to be performing a Gramm-Schmidt process on his components α_i . The

confusion probably arose because Hoffman & Kunze (1961) (Peusner's reference) used α_i to denote vectors.

It is not our purpose here to analyse Peusner's paper in detail. We would simply like to point out that "the Euclidean geometry of fluctuation-dissipation space" was well established by us several years earlier. Since then, the theory of the phenomenological calculus of description space (as we call the theory) has been extended both mathematically (to Riemannian manifold, Hilbert tensor spaces, . . .) and in terms of physical and biological applications (quantum mechanics, aging, relativity, . . .). In particular, in a second 1982 paper (Louie *et al.*, 1982) we constructed a geometry consistent with irreversible thermodynamics, where the constitutive parameters $\{\mathbf{a}^i\}$ lead to the metric tensor $\{L^{ij}\}$, from which the Onsager symmetry relations are immediately established. The metric form that corresponds to the Second Law is a direct consequence of the construction of a positive definite norm. As a contrast, Peusner assumes his (g_{ij}) is a metric by "physical requirement" (top of p. 135).

We urge the readers to consult our sequence of papers (loc. cit. and Louie, 1983; Louie & Richardson, 1983; Richardson & Louie, 1983, 1986; Louie & Richardson, 1986) for a solid foundation of the metric geometry of irreversible thermodynamics. In particular, it should become clear that the proper (and unique) metric associated with Peusner's fluctuation " $-\Delta S$ " is given in our formulation by the response vector $\mathbf{R} = \mathbf{a}_i J^i$ with the scalar "fluxes" $J^i = \alpha^i / \sqrt{2}$ and $g_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$. It should be noticed that the characterization of a dissipative system by a response tensor, \mathbf{R} , rather than by a vector, \mathbf{R} , allows the consideration of vector (not merely scalar) forces and fluxes. Finally, it must be pointed out that equation (32) of Richardson (1980) should read $\mathbf{R} : \mathbf{R} = (\mathbf{a}^i \cdot \mathbf{a}^j)(\mathbf{F}_i \cdot \mathbf{F}_j)$; the subsequent identification with the dissipation function is then trivial.

86 Dagmar Avenue,
Vanier, Ontario,
K1L 5T4, Canada

A. H. LOUIE

908 Middle Avenue, Apt. O,
Menlo Park, CA 94025, U.S.A.

I. W. RICHARDSON

(Received 22 September 1987, and in revised form 25 January 1988)

REFERENCES

- HOFFMAN, K. & KUNZE, R. (1961). *Linear Algebra*. Englewood Cliffs, NJ: Prentice-Hall.
 LOUIE, A. H. (1983). *Bull. Math. Biol.* **45**, 1029.
 LOUIE, A. H. & RICHARDSON, I. W. (1983). *Math. Modelling* **4**, 555.
 LOUIE, A. H. & RICHARDSON, I. W. (1986). *Math. Modelling* **7**, 227.
 LOUIE, A. H., RICHARDSON, I. W. & SWAMINATHAN, S. (1982). *J. theor. Biol.* **94**, 77.
 PEUSNER, L. (1986). *J. theor. Biol.* **122**, 125.
 RICHARDSON, I. W. (1980). *J. theor. Biol.* **85**, 745.
 RICHARDSON, I. W. & LOUIE, A. H. (1983). *J. theor. Biol.* **102**, 199.
 RICHARDSON, I. W. & LOUIE, A. H. (1986). *Math. Modelling* **7**, 211.
 RICHARDSON, I. W., LOUIE, A. H., & SWAMINATHAN, S. (1982). *J. theor. Biol.* **94**, 61.