Research Article

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On the Combined Use of Friction Matrices and Dissipation Potentials in Thermodynamic Modeling

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Abstract: Gradient flows and generalized gradient flows, associated with friction matrices and dissipation potentials, respectively, are usually regarded as two alternative possibilities to choose from in modeling irreversible time evolution in nonequilibrium thermodynamics. We here argue that these two possibilities actually need to be combined and we address a number of physical and mathematical issues associated with this task. Dimensional considerations provide important insights into these issues.

Keywords: GENERIC, dissipation potential, friction matrix, generalized gradient flow, dimensional analysis

1 Problem and questions

When the GENERIC (general equation for the nonequilibrium reversible-irreversible coupling) framework was presented and elaborated in [1, 2] more than 20 years ago, two alternative ways of writing the irreversible contribution to time evolution were offered in eqs. (4) and (13) of [1]:

\[ \frac{dx}{dt} = M \frac{\delta S}{\delta x} \]  

or

\[ \frac{dx}{dt} = \frac{\delta \Psi}{\delta (\delta S/\delta x)} \]  

Both formulations can be considered as gradient flows for the system variables x, generated by the gradient of the entropy S(x). In eq. (1), the friction matrix M is positive-semidefinite. In eq. (2), the dissipation potential Ψ is a convex real-valued function that has its minimum at 0, where Ψ(0) = 0 (for the origins of using dissipation potentials in irreversible thermodynamics, see [3, 4, 5, 6, 7]; see also the remarks in Section 2.9 of [8]). The potential Ψ can have an additional dependence on x, and also M usually depends on x. The notation \( \delta / \delta x \) indicates that we often deal with fields and functional derivatives; for discrete system variables, \( \delta / \delta x \) reduces to partial derivatives (see, for example, eqs. (10) and (11) below). The formulation of irreversible dynamics in terms of a dissipation potential is also known as generalized gradient flow (see [9] and references therein). In the following, we hence distinguish between gradient flows (1) and generalized gradient flows (2), or between gradient flows based on friction matrices and based on dissipation potentials.

The respective advantages of the formulations (1) and (2) have been discussed in the literature, in most detail in [10]. In particular, it has been shown that any generalized gradient flow can be rewritten as a gradient flow, but not vice versa [10]. The recent observation that not only gradient flows [11] but also generalized gradient flows [12] can be obtained from statistical mechanics puts the two formulations on a more equal footing, and they can actually be distinguished by the fluctuations naturally implied by them (for an alternative microscopic derivation of dissipation potentials from Hamiltonian dynamics see [13]). The purpose of

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this note is to show that a more relevant task is to combine these two formulations, not to choose between them. In particular, we address the following, closely related questions:

1. How can the strong formulation of energy conservation (energy degeneracy), which plays an important role in modeling irreversible dynamics in terms of gradient flows, be accommodated to generalized gradient flows?
2. What are the physical and mathematical implications of the fact that nonhomogeneous functions (dissipation potentials) can be evaluated only for dimensionless arguments?
3. Why should and how could the formulations (1) and (2) be combined in thermodynamic modeling?

The hydrodynamics of multicomponent fluids in the presence of chemical reactions is an example of a system where the combination of friction matrices (for transport) and dissipation potentials (for reactions) is advantageous (in particular, if one is interested in fluctuations [14]).

2 Decoupling of dissipative processes

In most applications, the modeling of irreversible processes is done in terms of friction matrices (see, for example, Appendix E of [15] or the more recent review articles [16, 17]). Moreover, the friction matrix \( M \) is usually assumed to be symmetric (for a more sophisticated discussion of the Onsager–Casimir symmetry properties of the friction matrix, see Sections 3.2.1 and 7.2.4 of [15], as well as [18]).

An important property of the friction matrix is the degeneracy of the energy \( E \),

\[
\frac{\delta E}{\delta x} \cdot M \frac{\delta A}{\delta x} = 0,
\]

(3)

for all sufficiently smooth functions \( A \), where the dot indicates the canonical pairing between gradient and tangent vectors. Equation (3) is a strong formulation of energy conservation because \( E \) is conserved not only for the physical time evolution generated by the entropy \( A = S \), but for all \( A \) (note that the dimensions of \( A \) do not matter in eq. (3)). This implies that \( M \) is degenerate because it possesses an eigenvector (the energy gradient \( \delta E/\delta x \)) with eigenvalue zero. As a consequence of this degeneracy of the energy, the friction matrix usually contains many off-diagonal elements. This feature reflects the fact that a dissipative process usually involves a number of variables and that a variable is often involved in several dissipative processes.

The straightforward generalization of the degeneracy condition (3) would be

\[
\frac{\delta E}{\delta x} \cdot \frac{\delta \Psi}{\delta (\delta A/\delta x)} = 0,
\]

(4)

for all \( A \). As long as the dissipation potential \( \Psi \) is a homogeneous function of its argument, usually of degree 2, this equation makes perfect sense, independent of the physical dimensions of the quantity \( A \). However, if \( \Psi \) is nonhomogeneous, for example an exponential function, then eq. (4) cannot make sense for all quantities \( A \) with varying physical dimensions. Such dimensional considerations are of no concern in the mathematical literature where dimensionless formulations are assumed from the outset (see, for example, Section 2.5 of [19] or Definition 2.5 of [20]). We should try to find out whether there are any deeper reasons why we need to consider dimensional issues in the context of dissipation potentials, but not in the context of friction matrices.

The left-hand side of eq. (3) can be considered as the definition of the bilinear and symmetric dissipative bracket of \( E \) and \( A \). For reasons of dimensional restrictions, the definition of a nonlinear bracket by the left-hand side of eq. (4) is much less useful. Meaningful nonlinear dissipation brackets do, however, appear in the single-generator framework of nonequilibrium thermodynamics developed by Beris and Edwards [21] (for a detailed comparison of the respective brackets see Section V.B of [2]; see also [22, 23, 24]). In that framework, the argument in the nonlinear part of the dissipation bracket always has dimensions of energy so that it can be made dimensionless in a consistent manner, unlike the arguments of varying physical dimensions occurring in a degeneracy condition.
For gradient flows based on friction matrices there is a simple way of decoupling dissipative processes. The basic idea is that friction matrices can typically be factorized as

$$M = CDC^T,$$  \hspace{1cm} (5)

where \(D\) is a positive-semidefinite symmetric matrix. One should not think of eq. (5) as a complete diagonalization of the symmetric matrix \(M\). Actually, the matrix \(D\) can be smaller than \(M\) and need not be diagonal, but typically is block-diagonal. Small blocks are natural, for example, when tensors are involved in viscous dissipation. The friction matrix inherits the symmetry and positive-semidefiniteness properties from \(D\). The normalization of \(C\) is not unique; any nonzero factor could be absorbed in \(D\).

As the size of the matrix \(D\) can be smaller than that of \(M\), the matrix \(C\) is not square. In particular, \(D\) can be chosen as a regular matrix. Dissipative processes can be decoupled by writing the full friction matrix as a sum of contributions of the form (5), where each of the contributions contains a small matrix \(D\) and is symmetric and positive-semidefinite (see, for example, Section 4.2.3 of [15]). With the factorization (5), the degeneracy property (3) becomes a property of \(C\) (that is, independent of the regular matrix \(D\)),

$$\frac{\delta E}{\delta x} \cdot C = 0.$$  \hspace{1cm} (6)

The matrix \(C\) describes how the various variables are involved in a dissipative process. It describes both how the driving forces associated with the system variables are combined into a driving force for the process (via \(C^T\)) and how the process changes all the variables (via \(C\)). In other words, the thermodynamic driving forces and the fluxes both involve the same matrix \(C\), which first narrows down to the essential driving force(s) of a particular process and then widens up the evolution caused by that process from the essential variables to all variables.

A central proposal of the present note is that the procedure of first focussing on essentials (via \(C^T\)) and then reconstructing the effect on all variables (via \(C\)) works in exactly the same symmetric manner for irreversible processes described by dissipation potentials. The proposed generalization of the decomposition (5) is

$$\Psi(x, \xi) = \psi(x, C^T(x) \xi),$$  \hspace{1cm} (7)

where \(\psi(x, \pi)\) is a dissipation potential in \(\pi = C^T(x) \xi\) and \(\xi\) eventually is to be interpreted as the entropy gradient \(\delta S/\delta x\). A similar construction for mapping a “process space” to a full tangent space was proposed in eq. (3.6) of [25] (cf. also, for example, eqs. (6) and (8) of [26] for isothermal chemical reactions, that is, without energy degeneracy). The dissipation potential \(\psi\) is the counterpart of the core matrix \(D\) in eq. (5), and the energy degeneracy then continues to be given by eq. (6) (without any dimensional issues arising for generalized gradient flows). The twofold role of \(C\) in the generalized setting becomes evident from the gradient (cf. the combination of eqs. (34) and (39a) of [10])

$$\frac{\delta \Psi(x, \xi)}{\delta \xi} = C(x) \left. \frac{\delta \psi(x, \pi)}{\delta \pi} \right|_{\pi = C^T(x) \xi}.$$  \hspace{1cm} (8)

The detailed implementation and further implications of the proposed generalization are elaborated in the following. This idea provides a full thermodynamic embedding of generalized gradient flows including conservation laws, most notably energy conservation.

3 Basic generalized gradient flows

Transport processes are typical examples of gradient flows that are naturally expressed in terms of friction matrices. Generalized gradient flows and dissipation potentials are encountered in modeling rare events.
For the example of a chemical reaction, rareness results from the difficulty of getting over a high (free) energy barrier separating two low-energy minima associated with the reactants and products (the corresponding transition rate has been determined in a classical paper by Kramers [27]). In the case of the Boltzmann equation, rareness results from the small probability of a collision between two particles in a rarified gas. Very different mechanisms lead to very similar equations for chemical reactions and the Boltzmann equation, both naturally described by dissipation potentials. The representation of chemical reactions, Boltzmann’s collision term and other jump processes by friction matrices is formally possible, but looks artificial [28, 29, 30, 31].

As indicated before, the dimensional analysis of generalized gradient flows (2) reveals some interesting issues. To allow for general nonlinear dependencies of the dissipation potential on the gradient $\xi = \delta S/\delta x$, this gradient should be dimensionless. Entropies can easily be made dimensionless by dividing them by the Boltzmann constant $k_B$, which may be considered as the microscopic unit of entropy. The important physical message is that we are led to counting microstates rather than working with a macroscopic entropy. We furthermore would like the variables $x$ to be dimensionless. Natural candidates for dimensionless variables are occupation numbers associated with a discrete set of states which, by proper normalization, may be considered as probabilities. Finally we should remember that the notation $\delta S/\delta x$ implies that, in general, we deal with functional derivatives. Our dimensional analysis suggests that, for spatially resolved systems, we should not consider entropies per unit volume but rather the entropies associated with particles or some discrete degrees of freedom. These conclusions are consistent with the statistical mechanics based on a fluctuation–dissipation relation between generalized gradient flows and Markov processes satisfying a large-deviation principle, where finding the intensity of the stochastic fluctuations requires a “correct counting” of microstates [9, 12]. In other words, the dimensional issues reveal that large fluctuations and hence also generalized gradient flows are intimately tied to statistical considerations (or “correct counting”), whereas gradient flows are associated with small fluctuations and can be handled in a purely phenomenological way.

The decomposition (7) reduces the problem of dimensionless $\xi$ to dimensionless $\pi$, which typically is a (much) smaller list of variables. One may think of the variables $\pi_k$ as the subset of thermodynamic driving forces for some probabilities $p_k$ that can be extracted from the full list of system variables $x$. The variables $p_k$ and $\pi_k$ represent the core of a dissipative process.

The general form of dissipation potentials for Markov jump processes with detailed balance is given by [32]

$$\psi(x, \pi) = \sum_{k,l} R_{kl}(x) \left[ e^{(n_l-n_k)/2} + e^{(n_l-n_k)/2} - 2 \right],$$  \hspace{1cm} (9)

with positive rate functions $R_{kl}(x)$, which can be taken as symmetric in $k$ and $l$. For $k = l$, the term in square brackets in eq. (9) vanishes so that the rates $R_{kk}(x)$ need not be defined. The dissipation potential (9) possesses the derivatives

$$\frac{\partial \psi(x, \pi)}{\partial \pi_k} = \sum_l R_{kl}(x) \left[ e^{(n_l-n_k)/2} - e^{(n_l-n_k)/2} \right].$$  \hspace{1cm} (10)

If interpreted as a gradient flow for probabilities, eq. (10) is the general evolution equation for the (transition) probabilities $p_k$ of a Markov process on a discrete state space in a thermodynamic formulation highlighting detailed balance. After summing over $k$, the symmetry of $R_{kl}(x)$ implies the condition $\sum_k \partial \psi(x, \pi)/\partial \pi_k = 0$, which reflects the conservation of the total probability, $\sum_k p_k = 1$. The nonnegative total dimensionless entropy production rate is given by

$$\sigma = \xi \cdot \frac{\partial \psi(x, \xi)}{\partial \xi} = \pi \cdot \frac{\partial \psi(x, \pi)}{\partial \pi} = \sum_{k,l} R_{kl}(x)(\pi_k - \pi_l)e^{(n_k-n_l)/2}.$$  \hspace{1cm} (11)

The dissipation potential (9) represents the basic generalized gradient flows to be used as the core part in the decomposition (7). In the next section, this idea is elaborated in the context of a specific example.
4 Example: A chemical reaction

In order to illustrate the decomposition (7) of the dissipation potential, we consider a simple reaction among three gases (under normal conditions),

\[ \text{N}_2 + 3 \text{H}_2 \rightleftharpoons 2 \text{NH}_3. \] (12)

Three different species of molecules are involved in this reaction (nitrogen, hydrogen, ammonia), and the corresponding stoichiometric coefficients are \( \nu_1 = -1, \nu_2 = -3 \) and \( \nu_3 = 2 \) (by standard convention, stoichiometric coefficients are negative for reactants and positive for products). We neglect flow and diffusion effects and use the state variable \( x = (\rho_1, \rho_2, \rho_3, s) \) consisting of the species mass densities \( \rho_1(r), \rho_2(r), \rho_3(r) \) and the total entropy density \( s(r) \). The masses of the different molecules are given by \( m_1, m_2 \) and \( m_3 \), respectively. The total energy \( E \) consists only of internal energy, the density of which is given by the local equilibrium relation \( \epsilon(\rho_1, \rho_2, \rho_3, s) \). The energy gradient takes the simple form

\[ T = \frac{\delta E}{\delta s} = \frac{\partial \epsilon}{\partial s}, \quad \mu_j = \frac{\delta E}{\delta \rho_j} = \frac{\partial \epsilon}{\partial \rho_j}, \quad \tilde{\mu}_j = \frac{\rho_j \mu_j}{k_B T}, \] (13)

where \( T \) is the temperature, \( \mu_j \) is the chemical potential per unit mass of species \( j \), and \( \tilde{\mu}_j \) is the dimensionless chemical potential per particle of species \( j \). As the entropy density is among the variables \( x \), the entropy gradient takes the simple form

\[ \frac{\delta S}{\delta x} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \] (14)

As the components of \( \delta S/\delta x \) are dimensionless, any nonhomogeneous function of these components can easily be evaluated. However, the same function could in general not be evaluated for the components of \( \delta E/\delta x \) given in eq. (13).

A chemical reaction involves two states separated by an energy barrier, one associated with the reactants \((k = 1)\) and the other one associated with the products \((k = 2)\). Following the general ideas of the preceding sections, we introduce two probabilities \( p_1, p_2 \) with \( p_1 + p_2 = 1 \) as new variables. Ideally, one would initially have only reactants in the right proportions (given by the stoichiometric coefficients). We would then have

\[ \rho_1 = m_1 \nu_1 \ n \ p_1, \quad \rho_2 = m_2 \nu_2 \ n \ p_2, \quad \rho_3 = m_3 \nu_3 \ n \ p_2, \] (15)

for the mass densities in terms of the probability \( p_1 \) for finding reactants and \( p_2 = 1 - p_1 \) for products, where \( n \) could be interpreted as the initial number density of nitrogen molecules (or one third of the initial number density of hydrogen molecules). More generally, we assume

\[ dp_1 = -m_1 \nu_1 \ n \ dp_1, \quad dp_2 = -m_2 \nu_2 \ n \ dp_1, \quad dp_3 = m_3 \nu_3 \ n \ dp_2. \] (16)

The number density \( n \) depends on the availability of the various species and the resulting possibilities of the reaction to go in the one or other direction. Knowing how changes of \( p_1 \) and \( p_2 \) affect the changes of the mass densities, we can now identify the matrix \( C \) in the decomposition (7),

\[ C = \begin{pmatrix} -m_1 \nu_1 & 0 \\ -m_2 \nu_2 & 0 \\ 0 & m_3 \nu_3 \\ k_B (\tilde{\mu}_1 \nu_1 + \tilde{\mu}_2 \nu_2) & -k_B \tilde{\mu}_3 \nu_3 \end{pmatrix}, \] (17)

where the last row of \( C \) follows from the energy degeneracy (6) and the factor of \( n \) is omitted (or reintroduced) in going from properties per unit volume to properties per particle (or vice versa). The dimensionless thermodynamic forces are given by

\[ \pi = C^T \xi = C^T \frac{1}{k_B} \frac{\delta S}{\delta x} = \begin{pmatrix} \tilde{\mu}_1 \nu_1 + \tilde{\mu}_2 \nu_2 \\ -\tilde{\mu}_3 \nu_3 \end{pmatrix}, \] (18)
which implies

\[ \pi_1 - \pi_2 = \tilde{\mu}_1 \nu_1 + \tilde{\mu}_2 \nu_2 + \tilde{\mu}_3 \nu_3. \]  

(19)

The evolution equation

\[ \frac{dx}{dt} = nC \left( \begin{array}{c} -m_1 \nu_1 \\ -m_2 \nu_2 \\ -m_3 \nu_3 \\ k_B (\tilde{\mu}_1 \nu_1 + \tilde{\mu}_2 \nu_2 + \tilde{\mu}_3 \nu_3) \end{array} \right) \frac{dp_1}{dt}, \]  

(20)

together with eq. (19) and the simplest special case of eq. (10),

\[ \frac{dp_1}{dt} = R_{12}(x) \left[ e^{(n_1 - n_2)/2} - e^{-(n_1 - n_2)/2} \right], \]  

(21)

reproduces the results of Section V.B of [2], where the chemical reaction (12) has been discussed in terms of a friction matrix. According to eq. (20), mass conservation can be expressed as

\[ \begin{pmatrix} 1 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} -m_1 \nu_1 \\ -m_2 \nu_2 \\ -m_3 \nu_3 \\ k_B (\tilde{\mu}_1 \nu_1 + \tilde{\mu}_2 \nu_2 + \tilde{\mu}_3 \nu_3) \end{pmatrix} \begin{pmatrix} \frac{dp_1}{dt} \\ \frac{dp_1}{dt} \\ \frac{dp_1}{dt} \end{pmatrix} = 0, \]  

(22)

and hence originates from the properties of \( C \).

We finally address the question where the anticipated statistical considerations and “correct counting” matter in the generalized gradient formulation of the chemical reaction (12). For ideal gases, the dimensionless chemical potentials in eq. (19) are of the form (see, e.g., eq. (7.2.4) of [33])

\[ \tilde{\mu}_j = \ln \left( \frac{\lambda_j(T)}{n_j} \right), \]  

(23)

with the number densities \( n_j = \rho_j/m_j \) and the thermal wave length

\[ \lambda_j(T) = \frac{h}{\sqrt{2\pi m_j k_B T}}, \]  

(24)

where \( h \) is Planck’s constant. For the ideal chemical potentials (23), eqs. (19) and (21) lead to the usual kinetic equations in terms of \( n_j^\nu \). The statistical considerations and “correct counting” are contained in the concrete form (23) of the chemical potentials with the explicit functions \( \lambda_j(T) \) given in eq. (24), where the occurrence of Planck’s constant signals the relevance of quantum statistical mechanics even for ideal gases (also for the “correct Boltzmann counting” required to resolve Gibbs’ paradox). For real gases, so-called activities are introduced to describe deviations from ideal chemical reactions, and Monte Carlo simulation methods for obtaining chemical potentials (or entropies), for example based on particle insertion [33, 34], thermodynamic integration [33], or scanning [35], always provide deviations from ideal behavior. Therefore, “correct counting” for ideal gases is essential for all ways of determining chemical potentials and hence has a crucial influence also on the description of chemical reactions among real gases by generalized gradient flows.

5 Concluding remarks

We have proposed a thermodynamic embedding of generalized gradient flows (based on dissipation potentials) that allows us to provide a strong formulation of energy conservation. Further conservation laws can be implemented in the same way. The proposed procedure relies on an embedding matrix for each dissipative process that simultaneously (i) extracts the relevant thermodynamic driving force or forces from the full entropy gradient and (ii) determines the changes of all system variables resulting from the dissipative pro-
cess. For the quadratic dissipation potentials associated with friction matrices, the proposed procedure is consistent with a previously proposed factorization of friction matrices.

Through the generalized embedding, the superposition of any number of dissipative processes becomes straightforward by adding the corresponding dissipation potentials. In particular, dissipative processes described by friction matrices and by dissipation potentials can be combined. The role of dimensional restrictions in generalized gradient flows has been related to the necessity of “correct counting” in the determination of entropy and fluctuations in statistical mechanics.

The present development is focused entirely on the irreversible contribution to time evolution. In the spirit of GENERIC, reversible contributions, which are generated by energy by means of a Poisson bracket, can be added easily [1, 2, 15, 36].

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