


Metriplectic four-bracket algorithm for constructing thermodynamically consistent dynamical systems

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A unified thermodynamic algorithm is presented for constructing thermodynamically consistent dynamical systems, i.e., systems that have Hamiltonian and dissipative parts that conserve energy while producing entropy. The algorithm is based on the metriplectic 4-bracket given in Morrison and Updike [Phys. Rev. E **109**, 045202 (2024)]. A feature of the unified thermodynamic algorithm is the force-flux relation $\mathbf{J}^\alpha = -L^{\alpha\beta} \nabla(\delta H/\delta \xi^\beta)$ for phenomenological coefficients $L^{\alpha\beta}$, Hamiltonian H , and dynamical variables ξ^β . The algorithm is applied to the Navier-Stokes-Fourier, the Cahn-Hilliard-Navier-Stokes, and Brenner-Navier-Stokes-Fourier systems, and significant generalizations of these systems are obtained.

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I. INTRODUCTION

Metriplectic dynamics was established in the 1980s [1–3] to provide a framework for describing joined Hamiltonian and dissipative dynamics with the property that thermodynamic consistency is guaranteed. (See [4–7] for different attempts at incorporating dissipation in a framework.) Thermodynamic consistency means the joined Hamiltonian and dissipative system conserves energy, consistent with the first law of thermodynamics, and produces entropy, consistent with the second law.

In 1997, the name GENERIC was proposed [8,9] for a framework that is equivalent to metriplectic dynamics (see page 11 of [10]). In a sequence of works [8,9,11] these authors were the first to explicitly incorporate ideas from nonequilibrium thermodynamics (e.g., [12]) into the framework. Specifically, Onsager’s reciprocal relations [13,14] were employed to ensure entropy production. More recently, the same connection between nonequilibrium thermodynamics theory and metriplectic dynamics was made in [15] for a general class of magnetofluid models and, more generally in [10], where the metriplectic 4-bracket, a convenient quantity for constructing thermodynamically consistent systems, was introduced.

In the theory of nonequilibrium thermodynamics, it is assumed that the fluxes, say \mathbf{J}^α , are typically linear functions of thermodynamic forces (sometimes called *affinities*), say \mathbf{X}_β ; i.e.,

$$\mathbf{J}^\alpha = L^{\alpha\beta} \mathbf{X}_\beta, \quad (1)$$

where $L^{\alpha\beta}$ is a symmetric matrix, α and β are indices for the set of dynamical variables, and the repeated β index is to be summed.

In our previous work [16], we proposed an algorithm for constructing a metriplectic 4-bracket and, consequently, a means for producing thermodynamically consistent systems. This was done for a general Navier-Stokes Cahn-Hilliard system, a model for two-phase flow. The algorithm has the following four steps. (1) First, select a set of dynamical variables. (2) Next, select energy and entropy functionals, H and S , dependent on the dynamical variables, based on the physics of the phenomena to be described. (3) The third step is to obtain the noncanonical Poisson bracket [17] of the ideal (nondissipative) part of the theory, with the chosen entropy as a Casimir invariant. (4) The final step is to construct a metriplectic 4-bracket. We will refer to the algorithm as the “unified thermodynamic algorithm” or UT algorithm for short.

The present work differs from previous work by singling out a particular way to take step (4), one that has significant consequences. In previous works [10,16,18], step (4) relied on past experience and intuition. As with previous work, this final step of the UT algorithm makes use of the Kulkarni-Nomizu (K-N) product [19,20] of two operators M and Σ . However, the burden of determining the two operators is made algorithmic and leads to several desirable properties. For example, a preferred choice of thermodynamic forces and fluxes is obtained, which are seen to be related in a manner different from the Onsager reciprocal relations of Eq. (1), viz.,

$$\mathbf{J}^\alpha = -L^{\alpha\beta} \nabla(\delta H/\delta \xi^\beta), \quad (2)$$

where ξ^β are a specific set of dynamical variables from step (1) of the UT algorithm, H is the Hamiltonian as obtained from step (2), and $\delta H/\delta \xi^\beta$ is the functional derivative.

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Tensorial consistency and the Curie symmetry principle [12] follow automatically from Eq. (2). In addition, we will see that expression (2) is intimately connected to the distinctive physical roles played by M and Σ , which guide their determination. Another consequence of our new step (4) of the UT algorithm is an unambiguous distinction between thermodynamic variables that enter a system because of the assumption of local thermodynamic equilibrium from those that enter in the phenomenological coefficients. We also note that expression (2) can be further generalized [see Eq. (33) below] by replacing ∇ with any pseudodifferential operator that has an adjoint instead of a simple spatial gradient. This adjoint assumption is crucial for obtaining general classes of metriplectic 4-brackets.

Consequently, the algorithm can proceed using the inputs: the Hamiltonian functional H , the entropy functional S , and the unknown coefficients $L^{\alpha\beta}$. Specification of H requires a choice for the internal energy, a function of thermodynamic variables that determines the equations of state. This embodies the assumption of local thermodynamic equilibrium. The dependence of the phenomenological coefficients $L^{\alpha\beta}$ on thermodynamic variables, however, provides another challenge. They may come from experiments, dilute liquid/gas kinetic theory, the Green-Kubo formalism [12], or molecular dynamics simulations. We emphasize that the UT algorithm has the new feature of clearly distinguishing dependencies on dynamical and thermodynamic variables that arise from the forces determined by $\delta H/\delta \xi^\beta$ from those determined by phenomenological coefficients $L^{\alpha\beta}$.

A point regarding the UT algorithm that is not addressed here is why the K-N form is used at all. This is a deeper question which could be addressed by appealing to general principles of an underlying kinetic theory. The universality of the 4-bracket applicability, ranging from various collisional kinetic theories to a large variety of complex fluids, suggest that this might be possible.

This paper is structured as follows. In Sec. II, we provide an overview of the metriplectic framework, where foundational concepts are reviewed, starting with the Hamiltonian formalism (Sec. II A) and moving to the metriplectic 4-bracket formalism (Sec. II B). At the end of this section we discuss the critical features needed in order to develop a systematic method to build the metriplectic 4-bracket. In Sec. III, we focus on the derivation of the metriplectic 4-bracket. Here, a systematic approach to the theory is developed (Sec. III A), followed by a discussion on the relationship to nonequilibrium thermodynamics principles (Sec. III B). In Sec. IV, we present three examples to illustrate the application of the developed theory by applying the UT algorithm. Specifically, the Navier-Stokes-Fourier (NSF) system (Sec. IV A), the Cahn-Hilliard-Navier-Stokes (CHNS) system (Sec. IV B), and the Brenner-Navier-Stokes-Fourier (BNSF) system (Sec. IV C) are explored as cases demonstrating the theory's flexibility and general applicability. We observe that the NSF and BNSF systems are special cases of a general theory we develop. Finally, in Sec. V we briefly summarize and make a few comments about ongoing and future work.

II. OVERVIEW ON METRIPLECTIC FRAMEWORK

A. Hamiltonian formalism

Let us briefly recall the Hamiltonian formalism in infinite dimensions. The first step of the UT algorithm presented in [16] involves selecting a set of dynamical variables. It is preferable to choose conserved quantities as the variables. For example, in fluid dynamics, one might select the mass density, momentum density, and entropy density. In general, we consider the dynamics of classical field theories involving multi-component fields

$$\xi(\mathbf{z}, t) = (\xi^1(\mathbf{z}, t), \xi^2(\mathbf{z}, t), \dots, \xi^N(\mathbf{z}, t)) \quad (3)$$

defined on $\mathbf{z} = (z^1, z^2, \dots, z^n) \in \Omega$ for times $t \in \mathbb{R}$. Here, we use \mathbf{z} to be a label space coordinate with the volume element $d^n z$, but with the domain Ω unspecified. For example, in fluid mechanics Ω would be the three-dimensional domain occupied by the fluid and we will use $\mathbf{x} = (x^1, x^2, x^3)$ to indicate a point in Ω for this case. In general, we suppose that ξ^1, \dots, ξ^N can be real-valued scalars or densities defined on space-time $\Omega \times \mathbb{R}$, vector fields in the tangent or cotangent bundles of the manifold Ω , or even elements in its tensor bundle. Thus, for some α , ξ^α could be a scalar, a vector, or any tensorial quantity that is convenient for the system being described. We will forgo formal geometric considerations and suppose our infinite-dimensional phase space has coordinates $\xi = (\xi^1, \dots, \xi^N)$ and observables are functionals that map $\xi \mapsto \mathbb{R}$ at each fixed time. We will denote the space of such functionals by \mathcal{B} . Then a Poisson bracket is an antisymmetric bilinear operator

$$\{ \cdot, \cdot \} : \mathcal{B} \times \mathcal{B} \rightarrow \mathcal{B}, \quad (4)$$

where this bracket is assumed to satisfy the Jacobi identity, $\{ \{F, G\}, K \} + \{ \{K, F\}, G \} + \{ \{G, K\}, F \} = 0$, thereby providing a realization of a Lie algebra [see, e.g., [21] Chap. 14], and, in addition, fulfill the Leibniz rule. A general infinite-dimensional form of this bracket, for any given two functionals $F, G \in \mathcal{B}$, can be written as follows:

$$\{ F, G \} = \int_{\Omega} d^n z \int_{\Omega} d^n z' \mathcal{J}^{\alpha\beta} \frac{\delta F}{\delta \xi^\alpha(z)} \frac{\delta G}{\delta \xi^\beta(z')}, \quad (5)$$

where $\mathcal{J}^{\alpha\beta}(z, z')$ is a 2-tensor functional operator that is antisymmetric, with coordinate form given by the following integral kernel:

$$\mathcal{J}^{\alpha\beta}(z, z')[\xi] = \mathcal{J}(\mathbf{d}\xi^\alpha(z), \mathbf{d}\xi^\beta(z'))[\xi],$$

where α, β range over $1, 2, \dots, N$, and $\delta F/\delta \xi^\alpha, \delta G/\delta \xi^\beta$ are the functional derivatives (see, e.g., [17] for a formal review of these notions).

Upon inserting any functional of ξ , say an observable ξ^α , into the Poisson bracket its evolution is determined by

$$\partial_t \xi^\alpha = \{ \xi^\alpha, H \}, \quad (6)$$

where $H[\xi] \in \mathcal{B}$ is a Hamiltonian functional. Here and henceforth we use the shorthand $\partial_t = \partial/\partial t$ for the partial derivative with respect time and we will use an overdot to mean the total derivative d/dt , i.e. $\dot{F} = dF/dt$. For example, the evolution of the Hamiltonian functional is given by $\dot{H} = \{H, H\} = 0$ due to the antisymmetry of the bracket. We will also use the shorthand $\partial_i = \partial/\partial z^i$ for the partial derivative with respect to

the spatial variable z^i . Casimir invariants are special functionals \mathcal{C} that satisfy $\{F, \mathcal{C}\} = 0$ for any functional F , and thus are constants of motion for any Hamiltonian.

The second step of the UT algorithm is the selection of the Hamiltonian functional and a Casimir invariant to serve as the entropy. The choice of these functionals is based on the physics of the phenomena one wishes to describe. However, across all the cases we have examined, the Hamiltonian functional is the total energy of the system and the usual total entropy of the system is a Casimir invariant.

The construction of the noncanonical Poisson bracket (5) is the third step of the UT algorithm. Since the publication of [22], there is a huge literature on this for a variety of systems (e.g., [10,15,17,18,23–26] give Poisson brackets for a great many systems, including fluid dynamics, magneto-fluid dynamics, two-phase fluid dynamics, plasma kinetic theory, and so on).

B. Metriplectic 4-bracket formalism

Step (4), the final step of the UT algorithm, is the construction of the metriplectic 4-bracket. This construction was introduced in [10] to describe dissipative dynamics. We briefly recall the metriplectic 4-bracket description for infinite-dimensional systems. In this description, we consider the dynamics of classical field theories with multi-component fields, as presented in Eq. (3). We define the 4-bracket on functionals as

$$(\cdot, \cdot; \cdot, \cdot) : \mathcal{B} \times \mathcal{B} \times \mathcal{B} \times \mathcal{B} \rightarrow \mathcal{B}, \quad (7)$$

such that for any four functionals $F, K, G, N \in \mathcal{B}$ we have

$$(F, K; G, N) = \int_{\Omega} d^n z \int_{\Omega} d^n z' \int_{\Omega} d^n z'' \int_{\Omega} d^n z''' \hat{R}^{\alpha\beta\gamma\delta} \times \frac{\delta F}{\delta \xi^{\alpha}(z)} \frac{\delta K}{\delta \xi^{\beta}(z')} \frac{\delta G}{\delta \xi^{\gamma}(z'')} \frac{\delta N}{\delta \xi^{\delta}(z''')}, \quad (8)$$

where $\hat{R}^{\alpha\beta\gamma\delta}(z, z', z'', z''')$ is a 4-tensor functional operator with coordinate form given by the following integral kernel:

$$\begin{aligned} \hat{R}^{\alpha\beta\gamma\delta}(z, z', z'', z''')[\xi] \\ = \hat{R}(\mathbf{d}\xi^{\alpha}(z), \mathbf{d}\xi^{\beta}(z'), \mathbf{d}\xi^{\gamma}(z''), \mathbf{d}\xi^{\delta}(z'''))[\xi], \end{aligned}$$

where $\alpha, \beta, \gamma, \delta$ range over $1, 2, \dots, N$. The 4-bracket is assumed to satisfy the following properties:

(a) Linearity in all arguments, e.g., for all $\lambda \in \mathbb{R}$

$$(F + \lambda H, K; G, N) = (F, K; G, N) + \lambda(H, K; G, N) \quad (9)$$

(b) The algebraic symmetries

$$(F, K; G, N) = -(K, F; G, N), \quad (10)$$

$$(F, K; G, N) = -(F, K; N, G), \quad (11)$$

$$(F, K; G, N) = (G, N; F, K). \quad (12)$$

(c) Derivation in all arguments, e.g.,

$$(FH, K; G, N) = F(H, K; G, N) + (F, K; G, N)H. \quad (13)$$

Here, as usual, FH denotes point-wise multiplication.

One way to create a specific metriplectic 4-bracket that has the requisite symmetry properties from Eqs. (9)–(13) is by

using the Kulkarni-Nomizu (K-N) product [19,20]. (See also [27] for relevant theorems.) Given two symmetric operator fields, say Σ and M , the K-N product is defined as follows:

$$\begin{aligned} (\Sigma \wedge M)(dF, dK, dG, dN) = & \Sigma(dF, dG)M(dK, dN) \\ & - \Sigma(dF, dN)M(dK, dG) \\ & + M(dF, dG)\Sigma(dK, dN) \\ & - M(dF, dN)\Sigma(dK, dG). \end{aligned} \quad (14)$$

Thus, consistent with the bracket formulation of Eq. (8), we define a 4-bracket according to

$$(F, K; G, N) = \int_{\Omega} d^n z W (\Sigma \wedge M)(dF, dK, dG, dN), \quad (15)$$

where W is an arbitrary weight function, depending on ξ and z , that multiplies $\Sigma \wedge M$. For the general forms of the bilinear operators Σ and M , we refer to [10,16]; here, we omit the details for brevity.

The 4-bracket tool plays a crucial role in the dissipative description of dynamics, provided it satisfies certain properties which guarantee the thermodynamic consistency—namely, the first law (energy conservation) and the second law (entropy production). These properties are referred to as “*minimal metriplectic properties*”.

Let H be the Hamiltonian functional associated to the Poisson bracket (5) and S its Casimir invariant. As we mentioned previously, in the vast majority of infinite-dimensional dynamics, particularly in fluid dynamics, H and S present the total energy and the total entropy, respectively. Thus, the minimal metriplectic properties are the combination of the requisite symmetries (9)–(13) and the positive semi-definiteness in the following manner: The sectional curvature defined as $K(H, S) := (S, H; S, H)$ should be non-negative

$$K(H, S) \geq 0. \quad (16)$$

The 4-brackets arising from a K-N product (15), will have the minimal metriplectic proprieties if both Σ and M are positive. If one of Σ or M is positive definite, defining an inner product, then the sectional curvature satisfies $(S, H; S, H) \geq 0$ with equality if and only if $\delta S / \delta \xi \propto \delta H / \delta \xi$. The proofs of these results were first established in [10] for the finite-dimensional case and later extended to the infinite-dimensional case in [16].

Now, for any observable functional of ξ , say ξ^{α} , its dissipative evolution is prescribed by

$$\partial_t \xi^{\alpha} = (\xi^{\alpha}, H; S, H). \quad (17)$$

Thus, we have thermodynamic consistency because

$$\dot{H} = (H, H; S, H) \equiv 0, \quad (18)$$

$$\dot{S} = (S, H; S, H) = K(H, S) \geq 0, \quad (19)$$

where Eq. (18) follows from the antisymmetry condition of Eqs. (10) and (19) follow from Eq. (16), i.e., that the sectional curvature is non-negative.

We remind the reader, that the 4-bracket automatically gives metriplectic 2-brackets (see [10] for discussion), such as those in the early works [1–3] via $(F, G)_H = (F, H; G, H)$.

Because of the symmetries of the 4-bracket, \dot{H} will vanish for any H , as opposed to designing the earlier 2-brackets to make this happen for specific Hamiltonians.

In our previous work [16], the fourth and final step of the UT algorithm was achieved by constructing the 4-bracket via the K-N product using the following general forms for the bilinear operators Σ and M :

$$M(dF, dG) = F_{\xi^\alpha} A^{\alpha\beta} G_{\xi^\beta}, \quad (20)$$

$$\Sigma(dF, dG) = \mathcal{L}^{(\alpha)}(F_{\xi^\alpha}) \cdot B^{\alpha\beta} \cdot \mathcal{L}^{(\beta)}(G_{\xi^\beta}), \quad (21)$$

where we compactified our notation by defining $F_{\xi^\alpha} := \delta F / \delta \xi^\alpha$ and $F_\xi := (F_{\xi^1}, F_{\xi^2}, \dots, F_{\xi^N})$. Here, the repeated indices are to be summed, $A^{\alpha\beta}$ and $B^{\alpha\beta}$ are symmetric in $\alpha, \beta = 1, \dots, N$, i.e., $A^{\alpha\beta} = A^{\beta\alpha}$ and $B^{\alpha\beta} = B^{\beta\alpha}$, and $\mathcal{L}^{(\alpha)}$, for $\alpha \in \{1, \dots, N\}$, is contained within a general class of pseudodifferential operators on \mathcal{B} . We have placed parentheses around the upper index of $\mathcal{L}^{(\alpha)}$ to emphasize that this index is not to be summed. When a specific value is placed in this slot there is no confusion and the parentheses will be dropped. We will see later that the parameters $A^{\alpha\beta}$ and $B^{\alpha\beta}$ could be scalars, 2-tensors, 3-tensors or even 4-tensors, depending on the tensorial character of ξ^α and the type of dissipation phenomena. The “.” of Eq. (21) then symbolizes the appropriate contractions.

This final step of the UT algorithm, as implemented in the previous works [10,16,18], has two avenues for criticism. First, in the examples of previous works, in particular for the NSF and CHNS systems, the definitions of M and Σ were not established in a systematic or methodological way. Rather, they were engineered to give desired results. Second, since we aim to develop a general dissipative dynamics formalism, independently of specification of the thermodynamics, it is reasonable that quantities should depend only on the selected set of dynamical variables, with the exception of coefficients of phenomenological laws. For example, in previous works, various factors of $1/T$ were inserted in various places in an ad hoc manner. Is this inserted temperature determined by the internal energy function of H or is it some other phenomenological assumption?

In Sec. III A, we will propose an unambiguous method for choosing the operators M and Σ , and thereby overcome these criticisms by a direct construction of the metriplectic 4-bracket. This approach is general and applicable to a broad range of infinite-dimensional systems. Various types of fluid dynamics, magnetofluid dynamics, two-phase fluid flows, and so on, are particular cases. We will show how our construction can significantly generalize systems in the literature.

III. DERIVATION OF METRIPLECTIC 4-BRACKETS

A. Systematic development of the theory

In this section we give our method for constructing the metriplectic 4-bracket. Thus, as discussed in Sec. II B, the UT algorithm becomes complete if we accomplish the final step by selecting the bilinear symmetric operators M and Σ of the K-N product. We provide a direct procedure for making these selections.

En route to our goal, we make some notational choices. In the first step of the UT algorithm, the selected set of dy-

namical variables defined on space-time $\Omega \times \mathbb{R}$ was defined as follows:

$$\xi(\mathbf{z}, t) = (\xi^1(\mathbf{z}, t), \xi^2(\mathbf{z}, t), \dots, \xi^N(\mathbf{z}, t)), \quad (22)$$

where we previously commented that it is preferable to choose the ξ^α to be densities. To be more specific, here we suppose $\xi^1(\mathbf{z}, t), \xi^2(\mathbf{z}, t), \dots, \xi^{N-1}(\mathbf{z}, t)$ satisfy conservation laws and the last component, ξ^N , represents the entropy density, i.e., the entropy per unit volume. In practice the various ξ^α besides the entropy ξ^N may, based on the physical properties under consideration, have particular tensorial qualities, e.g., they may be scalars, vectors, or tensors or pseudo-tensors of arbitrary rank. To avoid a clutter of notation, we will not be explicit about this tensorial character, but strive for a notation that makes it clear how to proceed in particular cases. The examples of Sec. IV should help clarify this. We also assume Ω denotes an arbitrary domain of \mathbb{R}^n with $\partial\Omega$ being its boundary. For convenience, we will omit the incremental volume element $d^n z$ for integrations over Ω , i.e., $\int_\Omega = \int_\Omega d^n z$. We assume strong boundary conditions such that all integrations by parts produce vanishing boundary terms.

Given our choice of ξ^N as the entropy density, the total entropy is evidently given by the following:

$$S[\xi] = \int_\Omega \xi^N. \quad (23)$$

This functional is required to be a Casimir invariant of the noncanonical Poisson bracket $\{\cdot, \cdot\}$, which one is assumed to have found in the third step of the UT algorithm, i.e.,

$$\{F, S\} = 0, \quad \forall F. \quad (24)$$

The Hamiltonian functional H associated to the noncanonical Poisson bracket $\{\cdot, \cdot\}$ is given by

$$H[\xi] = \int_\Omega h, \quad (25)$$

where h , the Hamiltonian density, in general depends on all the variables $\xi^1, \xi^2, \dots, \xi^N$. We will take H to be the total energy, as is indeed the case for the examples mentioned in Sec. II A. The evolution of the dynamical variables in the ideal case, i.e., when dissipation is not included, is given by

$$\partial_t \xi^\alpha = \{\xi^\alpha, H\}, \quad \alpha = 1, 2, \dots, N. \quad (26)$$

Now it remains to add to Eq. (26) the dissipative evolution, which has the following natural combined form:

$$\partial_t \xi^\alpha = \{\xi^\alpha, H\} + \mathcal{L}^{(\alpha)} \cdot \mathbf{J}^\alpha, \quad \alpha = 1, \dots, N-1, \quad (27)$$

$$\partial_t \xi^N = \{\xi^N, H\} + \mathcal{L}^{(N)} \cdot \mathbf{J}^N + \mathbf{Z}_\alpha \cdot \tilde{\mathcal{L}}^{\alpha\beta} \cdot \mathbf{Z}_\beta. \quad (28)$$

Equation (27) is the sum of two conservative terms, the first being Hamiltonian while the second is dissipative. In this second expression α is not summed, but a particular operator $\mathcal{L}^{(\alpha)}$ may act on each flux \mathbf{J}^α . Recall, this was the purpose of the parenthesis. If ξ^α were a rank m tensor, then usually \mathbf{J}^α would be of rank $m+1$ with the contraction indicated by “.” providing tensorial consistency. However, we leave open the possibility that $\mathcal{L}^{(\alpha)}$ may contribute to tensorial consistency. For usual nonequilibrium thermodynamics $\mathcal{L}^{(\alpha)} = -\nabla$, for all α , and the conservative form of Eq. (27) is manifest.

Equation (28) similarly has conservative terms, but the addition of the last term is responsible for entropy production. Because ξ^N is a scalar density, \mathbf{J}^N is a vector and the contractions of $\mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta$ between some “vector fields” \mathbf{Z}_α and a quantity $\tilde{L}^{\alpha\beta}$ produces the correct tensorial form. Since the entropy production must be guaranteed, we assume $\tilde{L}^{\alpha\beta}$ is symmetric and positive semidefinite, giving

$$\dot{S} = \int_{\Omega} \mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta =: \int_{\Omega} \dot{\sigma}^{\text{prod}} \geq 0. \quad (29)$$

The construction above is similar to that presented in [[15], see page 14], in order to construct a general form of metriplectic 2-bracket. However, there the pseudodifferential operators were all taken to be spatial gradients, i.e., $\mathcal{L}^{(\alpha)} := -\nabla$. Here, we generalize this by supposing each operator $\mathcal{L}^{(\alpha)}$ has an adjoint $\mathcal{L}_*^{(\alpha)}$ defined with respect to the standard inner product, i.e., $(f, g) = \int_{\Omega} f g$, which of course is the case for ∇ , where $\nabla_* = -\nabla$.

What we have accomplished so far is the first step of the *analysis-synthesis* method, the *analysis phase*. With this method we work backwards from the desired form of the dynamical Eqs. (27) and (28). In the second step, the *synthesis phase*, we determine explicitly the quantities \mathbf{J}^α , \mathbf{Z}_α , and $\tilde{L}^{\alpha\beta}$. We will show that these quantities are expressed in terms of the functional derivatives of the Hamiltonian H_{ξ^α} . To be clear, we remind the reader that the goal of this analysis-synthesis process is to construct the operators M and Σ .

Given any functional $F[\xi]$, we have the basic identity

$$\dot{F}[\xi] = \int_{\Omega} \frac{\delta F}{\delta \xi^\alpha} \partial_t \xi^\alpha. \quad (30)$$

This follows upon assuming Ω is fixed and boundary terms vanish, which we have assumed throughout. Applying Eq. (30) to H and using our notation $H_{\xi^\alpha} = \delta H / \delta \xi^\alpha$, we obtain upon substitution of Eqs. (27) and (28)

$$\begin{aligned} \dot{H}[\xi] &= \int_{\Omega} H_{\xi^\alpha} \mathcal{L}^{(\alpha)} \cdot \mathbf{J}^\alpha + H_{\xi^N} \mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta \\ &= \int_{\Omega} \mathbf{J}^\alpha \cdot \mathcal{L}_*^{(\alpha)} H_{\xi^\alpha} + H_{\xi^N} \mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta. \end{aligned} \quad (31)$$

To ensure energy conservation, Eq. (31) must vanish. Simple and natural choices that achieve this end are the following generalized force-flux relations:

$$\mathbf{Z}_\alpha = \mathcal{L}_*^{(\alpha)} H_{\xi^\alpha}, \quad (32)$$

$$\mathbf{J}^\alpha = -H_{\xi^N} \tilde{L}^{\alpha\beta} \mathcal{L}_*^{(\beta)} H_{\xi^\beta}. \quad (33)$$

To understand these formulas, consider the standard case where $\mathcal{L}^{(\alpha)} = -\nabla$ for all α . This gives the force-flux relations,

$$\mathbf{Z}_\alpha = \nabla H_{\xi^\alpha}, \quad (34)$$

$$\mathbf{J}^\alpha = -H_{\xi^N} \tilde{L}^{\alpha\beta} \nabla H_{\xi^\beta} = -L^{\alpha\beta} \nabla H_{\xi^\beta}, \quad (35)$$

where in the second equality of Eq. (35) we have made comparison with Eq. (2). Thus,

$$L^{\alpha\beta} = H_{\xi^N} \tilde{L}^{\alpha\beta} \quad (36)$$

and we see that the $L^{\alpha\beta}$ of Eq. (2) is not the same as $\tilde{L}^{\alpha\beta}$ of Eq. (28). If the Hamiltonian obtains its σ dependence in the

standard way via an internal energy function, we will see that these quantities differ by a factor of T , i.e.,

$$\tilde{L}^{\alpha\beta} = L^{\alpha\beta} / T. \quad (37)$$

Now, we are in position to determine the M and Σ of the K-N product and hence the metriplectic 4-bracket. We are led to the following choices:

$$M(dF, dG) = F_{\xi^N} G_{\xi^N}, \quad (38)$$

$$\begin{aligned} \Sigma(dF, dG) &= \mathcal{L}_*^{(\alpha)}(F_{\xi^\alpha}) \tilde{L}^{\alpha\beta} \mathcal{L}_*^{(\beta)}(G_{\xi^\beta}) \\ &= \mathcal{L}_*^{(\alpha)}(F_{\xi^\alpha}) \frac{L^{\alpha\beta}}{H_{\xi^N}} \mathcal{L}_*^{(\beta)}(G_{\xi^\beta}). \end{aligned} \quad (39)$$

Here, we have chosen the simplest form for M , which singles out entropy, and makes the meaning of Σ perspicuous.

Constructing the 4-bracket with these choices of M and Σ , according to

$$(F, K; G, N) = \int_{\Omega} (\Sigma \wedge M)(dF, dK, dG, dN), \quad (40)$$

gives Eqs. (27) and (28), in metriplectic form, viz.,

$$\partial_t \xi^\alpha = \{ \xi^\alpha, H \} + (\xi^\alpha, H; S, H), \quad \forall \alpha = 1, \dots, N. \quad (41)$$

Manifestly, Eq. (18) is satisfied and we have for (19)

$$\begin{aligned} \dot{S} &= (S, H; S, H) = K(H, S) = \int_{\Omega} \Sigma(dH, dH) \\ &= \int_{\Omega} \mathcal{L}_*^{(\alpha)}(H_{\xi^\alpha}) \tilde{L}^{\alpha\beta} \mathcal{L}_*^{(\beta)}(H_{\xi^\beta}) \geq 0. \end{aligned} \quad (42)$$

Comparison with Eq. (29) reveals $\dot{\sigma}^{\text{prod}}$ becomes

$$\begin{aligned} \dot{\sigma}^{\text{prod}} &= \Sigma(dH, dH) = \mathcal{L}_*^{(\alpha)}(H_{\xi^\alpha}) \tilde{L}^{\alpha\beta} \mathcal{L}_*^{(\beta)}(H_{\xi^\beta}) \\ &= \mathcal{L}_*^{(\alpha)}(H_{\xi^\alpha}) \frac{L^{\alpha\beta}}{H_{\xi^N}} \mathcal{L}_*^{(\beta)}(H_{\xi^\beta}). \end{aligned} \quad (43)$$

Thus, the theory is complete once the phenomenological coefficients $L^{\alpha\beta}$ are determined. We reiterate that our construction clearly delineates between the phenomenological laws embodied in $L^{\alpha\beta}$ and the local thermodynamics contained in the Hamiltonian, e.g., in the internal energy function. Also, choosing M , as in Eq. (38), endows Σ with the physical meaning inherent in Eqs. (42) and (43), relating entropy production and sectional curvature.

We comment further on these coefficients in the context of nonequilibrium thermodynamics theory in Sec. III B.

B. Nonequilibrium thermodynamics theory

Many phenomena can be described by the idea that fluxes are caused by gradients of quantities, which are viewed as the thermodynamic forces. For example, Fourier's law relates heat flow to temperature gradients, Fick's law relates diffusion to concentration gradients, and in the Navier-Stokes equation momentum flux is related to velocity gradients. In nonequilibrium thermodynamics this is generalized by assuming fluxes are linear combinations of thermodynamic forces and, thereby, allowing for cross-effects. This is the essence of the Onsager reciprocal relations [13,14], which are

here represented by the force-flux relations of Eq. (1) (see, e.g., [12]).

For gaseous systems, an underlying kinetic theory can provide a justification for the phenomenological relations embodied in the $L^{\alpha\beta}$. This is the case for low-density gases, but, in general, such calculations are difficult or even prohibitive. However, many irreversible processes are empirically seen to be governed by linear relations between fluxes and forces [28] and, in this way, the $L^{\alpha\beta}$ are provided. However they are provided, our theory leaves open the possibility that they can depend on all the dynamical variables.

Returning to the theory developed in Sec. III A, we observe from Eq. (33) that the thermodynamic forcelike terms now take the new form $\mathcal{L}^{(\alpha)}H_{\xi^\alpha}$, where H is the Hamiltonian functional [cf. Eq. (2)]. In Sec. IV, we will confirm that our new form $\mathcal{L}^{(\alpha)}H_{\xi^\alpha}$ can match known examples and that our last step of the UT algorithm leading to the metriplectic 4-bracket provides a means for generalizing known examples and providing new thermodynamically consistent theories.

IV. EXAMPLES

In this section, we will give three examples. For all the examples, we consider the case where we have a single real-valued field variable, depending on one space- and one time-independent variable, $\xi(\mathbf{x}, t)$ where $\mathbf{x} = (x^1, x^2, x^3)$ is a Cartesian coordinate for a fluid contained in a volume Ω . Throughout the following, we use boldface to denote vectors, an over bar to denote rank-2 tensors, and a double over bar to denote rank-4 tensors.

A. Navier-Stokes-Fourier (NSF)

As a first example, we begin with the NSF system, which was previously considered in [2, 10, 16, 29]. En route, we find the algorithm produces a significantly more general system that contains the NSF as a special case.

First step of UT algorithm. We choose the set of fluid variables as follows:

$$\xi(\mathbf{x}, t) = (\rho(\mathbf{x}, t), \mathbf{m}(\mathbf{x}, t), \sigma(\mathbf{x}, t)), \quad (44)$$

where ρ is the mass density, $\mathbf{m} = \rho\mathbf{v}$ is the momentum density with \mathbf{v} being the Eulerian velocity field, and σ is the entropy density. Observe we have singled out the entropy density σ as the last variable, consistent with Eq. (22).

Second step of UT algorithm. Consistent with Eq. (23), we take the total entropy to be the integral of the last component

$$S = \int_{\Omega} \sigma. \quad (45)$$

A natural choice of Hamiltonian functional for NSF is

$$H = \int_{\Omega} \frac{|\mathbf{m}|^2}{2\rho} + \rho u(\rho, \sigma/\rho), \quad (46)$$

the sum of fluid kinetic energy and ρ times the specific internal energy u , which is known to be conserved by the NSF. More general Hamiltonians including, e.g., the gravitational force would be straightforward. The usual thermodynamic

relations are

$$p = \rho^2 \frac{\partial u}{\partial \rho} \quad \text{and} \quad T = \frac{\partial u}{\partial s}, \quad (47)$$

where the specific entropy $s = \sigma/\rho$. Alternatively, we can leave the Hamiltonian unspecified, i.e., let it be any functional $H[\rho, \mathbf{m}, \sigma]$; independent of its form, any H will be conserved by the metriplectic 4-bracket dynamics.

Third step of UT algorithm. The appropriate Poisson bracket is the so-called Lie-Poisson bracket given in Eq. [22]. For two functionals $F, G \in \mathcal{B}$ it is defined as follows:

$$\begin{aligned} \{F, G\} = & - \int_{\Omega} \mathbf{m} \cdot [F_{\mathbf{m}} \cdot \nabla G_{\mathbf{m}} - G_{\mathbf{m}} \cdot \nabla F_{\mathbf{m}}] \\ & + \rho [F_{\mathbf{m}} \cdot \nabla G_{\rho} - G_{\mathbf{m}} \cdot \nabla F_{\rho}] \\ & + \sigma [F_{\mathbf{m}} \cdot \nabla G_{\sigma} - G_{\mathbf{m}} \cdot \nabla F_{\sigma}], \end{aligned} \quad (48)$$

where S is a Casimir invariant, i.e., $\{S, F\} = 0$, for any functional F .

Fourth step of UT algorithm. To construct the metriplectic 4-bracket, we proceed with the systematic development presented in Sec. III A, viz., M and Σ are given by

$$M(dF, dG) = F_{\sigma} G_{\sigma}, \quad (49)$$

$$\Sigma(dF, dG) = \mathcal{L}_*^{(\alpha)}(F_{\xi^\alpha}) \frac{L^{\alpha\beta}}{H_{\sigma}} \mathcal{L}_*^{(\beta)}(G_{\xi^\beta}), \quad (50)$$

and the UT algorithm is complete up to the choices for $\mathcal{L}_*^{(\alpha)}$ and $L^{\alpha\beta}$. For any choices of these quantities, according to Eqs. (33) and (36), the 4-bracket using Eqs. (49) and (50) will be consistent with the following general expressions for the fluxes:

$$\begin{aligned} \mathbf{J}_{\rho} &= -L^{\rho\rho} \cdot \mathcal{L}_*^{\rho}(H_{\rho}) - L^{\rho\mathbf{m}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\rho\sigma} \cdot \mathcal{L}_*^{\sigma}(H_{\sigma}), \\ \bar{\mathbf{J}}_{\mathbf{m}} &= -L^{\mathbf{m}\rho} \otimes \mathcal{L}_*^{\rho}(H_{\rho}) - L^{\mathbf{m}\mathbf{m}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\mathbf{m}\sigma} \otimes \mathcal{L}_*^{\sigma}(H_{\sigma}), \\ \mathbf{J}_s &= -L^{\sigma\rho} \cdot \mathcal{L}_*^{\rho}(H_{\rho}) - L^{\sigma\mathbf{m}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\sigma\sigma} \cdot \mathcal{L}_*^{\sigma}(H_{\sigma}), \end{aligned} \quad (51)$$

where \mathbf{J}_{ρ} is the net mass flux, $\bar{\mathbf{J}}_{\mathbf{m}}$ is the momentum flux, and \mathbf{J}_s is the net entropy flux. Equation (51) shows how our choices of M and Σ , of Eqs. (49) and (50), respectively, produce a quite-general thermodynamically consistent system, one that significantly generalizes the NSF system. In fact, the 4-bracket that produces Eq. (51) is sufficiently general to produce the Brenner-Navier-Stokes system of Sec. IV C and the generalizations of the BNS that we describe there.

Now, we specialize and show that the general expressions for the fluxes of Eq. (51) reduce to those known for the NSF (see, e.g., [2, 12, 15]), viz.,

$$\mathbf{J}_{\rho} = 0, \quad \bar{\mathbf{J}}_{\mathbf{m}} = -\bar{\Lambda} : \nabla \mathbf{v}, \quad \mathbf{J}_s = -\frac{\bar{\kappa}}{T} \cdot \nabla T, \quad (52)$$

where \mathbf{J}_{ρ} is the net (vector) mass flux, $\bar{\mathbf{J}}_{\mathbf{m}}$ is the momentum flux (rank 2 tensor), and \mathbf{J}_s is the net (vector) entropy flux. In Eq. (52), $\bar{\kappa}$ is the thermal conductivity tensor, \bar{D} is the diffusion tensor, which along with $\bar{\kappa}$ is assumed to be a symmetric and positive definite 2-tensor, and $\bar{\Lambda}$ is the viscosity 4-tensor, the usual rank 4 isotropic Cartesian tensor given by

$$\Lambda_{ijkl} = \eta(\delta_{il}\delta_{jk} + \delta_{jl}\delta_{ik} - \frac{2}{3}\delta_{ij}\delta_{kl}) + \zeta\delta_{ij}\delta_{kl}, \quad (53)$$

with viscosity coefficients η and ζ and i, j, k , and l taking on values 1, 2, 3. In Eq. (52) and, henceforth, we use a single “.” to indicate neighboring contractions and we use the double dot convention as follows:

$$\begin{aligned} (\bar{\kappa} \cdot \nabla G_\sigma)_i &= \kappa_{ij} \partial_j G_\sigma \\ (\bar{\bar{\Lambda}} : \nabla \mathbf{m})_{ij} &= \Lambda_{ijkl} \partial_k m_l \\ (\epsilon : \nabla \mathbf{m})_i &= \epsilon_{ijk} \partial_j m_k, \end{aligned} \quad (54)$$

where repeated indices are summed over. We have added Eq. (54) for later use, when we have a double contraction with a 3-tensor ϵ .

To see how the fluxes of Eq. (52) emerge from our general expressions of Eq. (51), we set $\mathcal{L}_*^{(\alpha)} = \nabla$, for all α , and assume H is given by Eq. (46); therefore,

$$H_\sigma = T, \quad H_{\mathbf{m}} = \mathbf{v}, \quad H_\rho = -\frac{|\mathbf{m}|^2}{2\rho^2} - \frac{T\sigma}{\rho} + \frac{p}{\rho} + u, \quad (55)$$

and comparison of Eq. (51) with Eq. (52) reveals that the only nonzero phenomenological coefficients $L^{\alpha\beta}$ are the following:

$$L^{\mathbf{m}\mathbf{m}} = \bar{\bar{\Lambda}} \quad \text{and} \quad L^{\sigma\sigma} = \frac{\bar{\kappa}}{T}. \quad (56)$$

Thus, we immediately obtain Σ from Eq. (50) as

$$\begin{aligned} \Sigma(dF, dG) &= \nabla F_{\mathbf{m}} : \frac{L^{\mathbf{m}\mathbf{m}}}{H_\sigma} : \nabla G_{\mathbf{m}} + \nabla F_\sigma \cdot \frac{L^{\sigma\sigma}}{H_\sigma} \cdot \nabla G_\sigma \\ &= \nabla F_{\mathbf{m}} : \frac{\bar{\bar{\Lambda}}}{T} : \nabla G_{\mathbf{m}} + \nabla F_\sigma \cdot \frac{\bar{\kappa}}{T^2} \cdot \nabla G_\sigma \end{aligned} \quad (57)$$

which, together with the expression for M of Eq. (49), gives the 4-bracket

$$\begin{aligned} (F, K; G, N) &= \int_\Omega \frac{1}{T} [[K_\sigma \nabla F_{\mathbf{m}} - F_\sigma \nabla K_{\mathbf{m}}] : \bar{\bar{\Lambda}} : [N_\sigma \nabla G_{\mathbf{m}} - G_\sigma \nabla N_{\mathbf{m}}] \\ &\quad + \frac{1}{T} [K_\sigma \nabla F_\sigma - F_\sigma \nabla K_\sigma] \cdot \bar{\kappa} \cdot [N_\sigma \nabla G_\sigma - G_\sigma \nabla N_\sigma]]. \end{aligned} \quad (58)$$

Insertion of H of Eq. (46) and S of Eq. (45), yields the NSF dynamical system

$$\begin{aligned} \partial_t \rho &= \{\rho, H\} + (\rho, H; S, H) \\ &= -\mathbf{v} \cdot \nabla \rho - \rho \nabla \cdot \mathbf{v}, \end{aligned} \quad (59)$$

$$\begin{aligned} \partial_t \mathbf{v} &= \{\mathbf{v}, H\} + (\mathbf{v}, H; S, H) \\ &= -\mathbf{v} \cdot \nabla \mathbf{v} - \nabla p / \rho + \frac{1}{\rho} \nabla \cdot (\bar{\bar{\Lambda}} : \nabla \mathbf{v}), \end{aligned} \quad (60)$$

$$\begin{aligned} \partial_t \sigma &= \{\sigma, H\} + (\sigma, H; S, H) \\ &= -\mathbf{v} \cdot \nabla \sigma - \sigma \nabla \cdot \mathbf{v} + \nabla \cdot \left(\frac{\bar{\kappa}}{T} \cdot \nabla T \right) \\ &\quad + \frac{1}{T^2} \nabla T \cdot \bar{\kappa} \cdot \nabla T + \frac{1}{T} \nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v}. \end{aligned} \quad (61)$$

By construction we automatically have the entropy production

$$\dot{S} = (S, H; S, H) = \int_\Omega \dot{\sigma}^{\text{prod}} \geq 0, \quad (62)$$

where

$$\dot{\sigma}^{\text{prod}} = \nabla \mathbf{v} : \frac{\bar{\bar{\Lambda}}}{T} : \nabla \mathbf{v} + \nabla T \cdot \frac{\bar{\kappa}}{T^2} \cdot \nabla T.$$

It is important to note that the square of the temperature in the denominator of the coefficient $\bar{\kappa}/T^2$ in $\dot{\sigma}^{\text{prod}}$ has factors from different physical origins. One factor comes from the systematic theory, where temperature is defined as $T := H_\sigma$, while the second arises from the phenomenological law, specifically Fourier's law, where the heat flux is given by $\mathbf{q} = -\bar{\kappa} \nabla T / T$.

B. Cahn-Hilliard-Navier-Stokes (CHNS)

Various equations have been proposed for describing two-phase fluid flow by combining the physics of the Cahn-Hilliard equation [30] with that of the Navier-Stokes equations (see, e.g., [31–34] and references therein). In these CHNS models, the influence of a second phase of matter is included by adding a concentration variable that describes the second phase. In [16] we used the metrileptic 4-bracket formalism to obtain a general model that encompasses, corrects, and generalizes existing models. As in Sec. IV A, in this section we will proceed with the UT algorithm and obtain a very general thermodynamically consistent two-phase flow system.

First step of UT algorithm. To our set of fluid variables we add a variable \tilde{c} , which is a concentration per unit volume that describes the second phase. Thus, our dynamical variables are

$$\xi(\mathbf{x}, t) = (\rho(\mathbf{x}, t), \mathbf{m}(\mathbf{x}, t), \tilde{c}(\mathbf{x}, t), \bar{\sigma}(\mathbf{x}, t)), \quad (63)$$

where, again, the mixture of two phases is assumed to be contained in a volume Ω , with coordinate \mathbf{x} , and to the densities ρ , \mathbf{m} , and $\bar{\sigma}$ used (as in Sec. IV A) we add \tilde{c} . Again, we have singled out the entropy density $\bar{\sigma}$ as the last variable of ξ , consistent with Eq. (22). (Note, the reason for the bar will soon become clear.) The specific concentration associated with \tilde{c} is given by $c = \tilde{c} / \rho$.

Second step of UT algorithm. Again, consistent with Eq. (23), we take the total entropy to be the integral of the last component

$$S = \int_\Omega \bar{\sigma}. \quad (64)$$

It was shown in [16] that this simple entropy can be used instead of the complicated entropy expressions used in [31–34], which were modeled after the free energy of the Cahn-Hilliard equation.

We record here for later use the relationship between our simple entropy $\bar{\sigma}$ and the previous one, which we denote by $\bar{\sigma}$, viz.,

$$\bar{\sigma} = \sigma + \frac{\lambda_s}{2} \Gamma^2(\nabla c). \quad (65)$$

Here, the coefficient λ_s is a constant and the function Γ is a homogeneous function of degree unity, i.e.,

$$\Gamma(\lambda \mathbf{p}) = \lambda \Gamma(\mathbf{p}) \quad \text{for all } \lambda > 0. \quad (66)$$

Because Γ is a homogeneous function of degree unity we have

$$\Gamma(\mathbf{p}) = \mathbf{p} \cdot \boldsymbol{\zeta} := p_j \frac{\partial \Gamma(\mathbf{p})}{\partial p_j}, \quad (67)$$

where ξ is a homogeneous function of degree zero. The function Γ was shown in [35] to describe anisotropic weighted mean curvature effects due to anisotropic surface tension.

Any Hamiltonian $H[\rho, \mathbf{m}, \tilde{c}, \bar{\sigma}]$ would be possible, however, as also shown in [16], the price paid for a simplified entropy is the following complicated Hamiltonian:

$$H = \int_{\Omega} \frac{|\mathbf{m}|^2}{2\rho} + \rho u(\rho, \sigma/\rho, \tilde{c}/\rho) + \frac{\lambda_u}{2} \Gamma^2(\nabla(\tilde{c}/\rho)), \quad (68)$$

where in the second argument of the internal energy u we have inserted σ as a shorthand for the expression in terms of $\bar{\sigma}$, \tilde{c} , and ρ obtained upon inserting σ from Eq. (65). From this extensive internal energy function, we obtain the intensive thermodynamical variables, including the chemical potential as

$$p = \rho^2 \frac{\partial u}{\partial \rho}, \quad T = \frac{\partial u}{\partial s}, \quad \text{and} \quad \mu = \frac{\partial u}{\partial c}, \quad (69)$$

where now $s = \bar{\sigma}/\rho$ and recall $c = \tilde{c}/\rho$. The parameter λ_u is another constant that describes anisotropic surface energy effects. In the previous works, it was shown how the constants λ_s and λ_u are related to λ_f , a parameter that depends on the temperature according to

$$\lambda_f(T) = \lambda_u - T\lambda_s. \quad (70)$$

We take this as given, referring the reader to the previous works for explanation.

Third step of UT algorithm. The appropriate Poisson bracket, defined on two functionals $(F, G \in \mathcal{B})$ is that for the Gibbs-Euler system given in [16]. This bracket, which is a natural generalization of that given in [22], is given by

$$\begin{aligned} \{F, G\} = & - \int_{\Omega} \mathbf{m} \cdot [F_{\mathbf{m}} \cdot \nabla G_{\mathbf{m}} - G_{\mathbf{m}} \cdot \nabla F_{\mathbf{m}}] \\ & + \rho [F_{\mathbf{m}} \cdot \nabla G_{\rho} - G_{\mathbf{m}} \cdot \nabla F_{\rho}] \\ & + \bar{\sigma} [F_{\mathbf{m}} \cdot \nabla G_{\bar{\sigma}} - G_{\mathbf{m}} \cdot \nabla F_{\bar{\sigma}}] \\ & + \tilde{c} [F_{\mathbf{m}} \cdot \nabla G_{\tilde{c}} - G_{\mathbf{m}} \cdot \nabla F_{\tilde{c}}]. \end{aligned} \quad (71)$$

It is simple to verify that the S of Eq. (64) is a Casimir invariant of this bracket.

Fourth step of UT algorithm. To construct the metriplectic 4-bracket, we proceed as in Sec. IV A with the forms of M and Σ given by Eqs. (49) and (50), albeit with $\bar{\sigma}$ replacing σ in Eq. (49). Thus, the determination of our system is complete when we make choices for $\mathcal{L}_*^{(\alpha)}$ and the $L^{\alpha\beta}$. For any choices of these quantities, the 4-bracket constructed from M and Σ will be consistent with the following general expressions for the fluxes obtained from Eq. (2):

$$\begin{aligned} \mathbf{J}_{\rho} = & -L^{\rho\rho} \cdot \mathcal{L}_*^{\rho}(H_{\rho}) - L^{\rho\mathbf{m}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) \\ & - L^{\rho\sigma} \cdot \mathcal{L}_*^{\sigma}(H_{\bar{\sigma}}) - L^{\rho\tilde{c}} \cdot \mathcal{L}_*^{\tilde{c}}(H_{\tilde{c}}), \\ \bar{\mathbf{J}}_{\mathbf{m}} = & -L^{\mathbf{m}\rho} \otimes \mathcal{L}_*^{\rho}(H_{\rho}) - L^{\mathbf{m}\mathbf{m}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) \\ & - L^{\mathbf{m}\sigma} \otimes \mathcal{L}_*^{\sigma}(H_{\bar{\sigma}}) - L^{\mathbf{m}\tilde{c}} \otimes \mathcal{L}_*^{\tilde{c}}(H_{\tilde{c}}), \\ \mathbf{J}_c = & -L^{\tilde{c}\rho} \cdot \mathcal{L}_*^{\rho}(H_{\rho}) - L^{\tilde{c}\mathbf{m}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) \\ & - L^{\tilde{c}\bar{\sigma}} \cdot \mathcal{L}_*^{\sigma}(H_{\bar{\sigma}}) - L^{\tilde{c}\tilde{c}} \cdot \mathcal{L}_*^{\tilde{c}}(H_{\tilde{c}}), \\ \mathbf{J}_s = & -L^{\bar{\sigma}\rho} \cdot \mathcal{L}_*^{\rho}(H_{\rho}) - L^{\bar{\sigma}\mathbf{m}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) \\ & - L^{\bar{\sigma}\bar{\sigma}} \cdot \mathcal{L}_*^{\sigma}(H_{\bar{\sigma}}) - L^{\bar{\sigma}\tilde{c}} \cdot \mathcal{L}_*^{\tilde{c}}(H_{\tilde{c}}). \end{aligned} \quad (72)$$

Thus, we have obtained a quite-general class of thermodynamically consistent systems, one that generalizes a variety of existing CHNS systems, depending on the choice of H , $L^{\alpha\beta}$, and \mathcal{L}_*^{α} .

Now, we specialize and show that the general expressions for the fluxes of Eq. (72) reduce to those known for the CHNS. For example, if we choose $\mathcal{L}_*^{(\alpha)} = \nabla$, for all α , and H to be the expression of Eq. (68), then we obtain the CHNS system of Anderson *et al.* [31–33] (see also [16]). Using

$$\begin{aligned} H_{\rho} = & -\frac{|\mathbf{m}|^2}{2\rho^2} + u + \rho u_{\rho} - \left(\frac{\sigma}{\rho} - \frac{\lambda_s}{2\rho} \Gamma^2\right) u_s - \frac{\tilde{c}}{\rho} u_c \\ & + \frac{\tilde{c}}{\rho^2} \nabla \cdot (u_s \lambda_s \Gamma \xi) + \frac{\tilde{c}}{\rho^2} \nabla \cdot (\Gamma \xi \lambda_u), \end{aligned} \quad (73)$$

$$H_{\tilde{c}} = u_c + \frac{\lambda_s}{\rho} \nabla \cdot (u_s \Gamma \xi) - \frac{1}{\rho} \nabla \cdot (\lambda_s \Gamma \xi) =: \mu_{\Gamma}, \quad (74)$$

$$H_{\mathbf{m}} = \mathbf{v}, \quad H_{\bar{\sigma}} = u_s = T, \quad (75)$$

where, from Eq. (69), we defined $u_{\rho} := \partial u / \partial \rho = p / \rho$, $u_s := \partial u / \partial s = T$, and $u_c := \partial u / \partial c = \mu$. Upon setting all the $L^{\alpha\beta}$ to zero except

$$L^{\mathbf{m}\mathbf{m}} = \bar{\bar{\Lambda}}, \quad L^{\bar{\sigma}\bar{\sigma}} = \frac{\bar{\kappa}}{T}, \quad \text{and} \quad L^{\tilde{c}\tilde{c}} = \bar{D}. \quad (76)$$

Equations (72) for the fluxes reduce to the following forms:

$$\mathbf{J}_{\rho} = 0, \quad \bar{\mathbf{J}}_{\mathbf{m}} = -\bar{\bar{\Lambda}} : \nabla \mathbf{v}, \quad (77)$$

$$\mathbf{J}_c = -\bar{D} \cdot \nabla \mu_{\Gamma}, \quad \mathbf{J}_s = -\frac{\bar{\kappa}}{T} \cdot \nabla T, \quad (78)$$

where $\mu_{\Gamma} := \mu - \frac{1}{\rho} \nabla \cdot (\lambda_s \Gamma \xi)$ and \bar{D} is a rank-2 diffusion tensor. Equations are the known fluxes for the CHNS system of [31–33].

The metriplectic 4-bracket for this case, as determined by

$$M(dF, dG) = F_{\bar{\sigma}} G_{\bar{\sigma}}, \quad (79)$$

$$\begin{aligned} \Sigma(dF, dG) = & \nabla F_{\mathbf{m}} : \bar{\bar{\Lambda}} : \nabla G_{\mathbf{m}} + \nabla F_{\bar{\sigma}} \cdot \frac{\bar{\kappa}}{T^2} \cdot \nabla G_{\bar{\sigma}} \\ & + \nabla(F_{\tilde{c}}) \cdot \frac{\bar{D}}{T} \cdot \nabla(G_{\tilde{c}}), \end{aligned} \quad (80)$$

is

$$\begin{aligned} (F, K; G, N) = & \int_{\Omega} \frac{1}{T} \left[[K_{\bar{\sigma}} \nabla F_{\mathbf{m}} - F_{\bar{\sigma}} \nabla K_{\mathbf{m}}] : \bar{\bar{\Lambda}} : [N_{\bar{\sigma}} \nabla G_{\mathbf{m}} - G_{\bar{\sigma}} \nabla N_{\mathbf{m}}] \right. \\ & + \frac{1}{T} [K_{\bar{\sigma}} \nabla F_{\bar{\sigma}} - F_{\bar{\sigma}} \nabla K_{\bar{\sigma}}] \cdot \bar{\kappa} \cdot [N_{\bar{\sigma}} \nabla G_{\bar{\sigma}} - G_{\bar{\sigma}} \nabla N_{\bar{\sigma}}] \\ & \left. + [K_{\tilde{c}} \nabla F_{\tilde{c}} - F_{\tilde{c}} \nabla K_{\tilde{c}}] \cdot \bar{D} \cdot [N_{\tilde{c}} \nabla G_{\tilde{c}} - G_{\tilde{c}} \nabla N_{\tilde{c}}] \right]. \end{aligned} \quad (81)$$

Upon insertion of H given by Eq. (68) and S given by Eq. (64), using Eqs. (73), (74), and (75) with $S_{\bar{\sigma}} = 1$, the following CHNS system is produced:

$$\begin{aligned} \partial_t \rho = & \{\rho, H\} + (\rho, H; S, H) \\ = & -\mathbf{v} \cdot \nabla \rho - \rho \nabla \cdot \mathbf{v}, \end{aligned} \quad (82)$$

$$\begin{aligned} \partial_t \mathbf{v} = & \{\mathbf{v}, H\} + (\mathbf{v}, H; S, H) \\ = & -\mathbf{v} \cdot \nabla \mathbf{v} - \frac{1}{\rho} \nabla \cdot [(p - \lambda_f \Gamma^2 / 2) \bar{I} \\ & + \lambda_f \Gamma \xi \otimes \nabla c] + \frac{1}{\rho} \nabla \cdot (\bar{\bar{\Lambda}} : \nabla \mathbf{v}), \end{aligned} \quad (83)$$

$$\begin{aligned}\partial_t \tilde{c} &= \{\tilde{c}, H\} + (\tilde{c}, H; S, H) \\ &= -\mathbf{v} \cdot \nabla \tilde{c} - \tilde{c} \nabla \cdot \mathbf{v} + \nabla \cdot (\tilde{D} \cdot \nabla \mu_\Gamma^0),\end{aligned}\quad (84)$$

$$\begin{aligned}\partial_t \bar{\sigma} &= \{\bar{\sigma}, H\} + (\bar{\sigma}, H; S, H) \\ &= -\mathbf{v} \cdot \nabla \bar{\sigma} - \bar{\sigma} \nabla \cdot \mathbf{v}\end{aligned}\quad (85)$$

$$\begin{aligned}&+ \nabla \cdot \left(\frac{\bar{\kappa}}{T} \cdot \nabla T \right) + \frac{1}{T^2} \nabla T \cdot \bar{\kappa} \cdot \nabla T \\ &+ \frac{1}{T} \nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v} + \frac{1}{T} \nabla \mu_\Gamma \cdot \bar{D} \cdot \nabla \mu_\Gamma,\end{aligned}\quad (86)$$

where \bar{I} is the identity and recall ξ is defined in Eq. (67),

$$\mu_\Gamma := u_c + \frac{\lambda_s}{\rho} \nabla \cdot (u_s \Gamma \xi) - \frac{1}{\rho} \nabla \cdot (\lambda_s \Gamma \xi), \quad (87)$$

and \otimes is the usual tensor product $(\mathbf{w} \otimes \mathbf{v})_{ij} = w_i v_j$.

The total entropy is governed by the following:

$$\begin{aligned}\dot{S} &= (S, H; S, H) \\ &= \int_\Omega \frac{1}{T} \left[\nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v} + \frac{1}{T} \nabla T \cdot \bar{\kappa} \cdot \nabla T \right. \\ &\quad \left. + \nabla \mu_\Gamma \cdot \bar{D} \cdot \nabla \mu_\Gamma \right] \geq 0,\end{aligned}\quad (88)$$

whence it is seen to be produced.

As noted above, some previous approaches to modeling CHNS systems employed nonstandard entropy expressions [31–34]. In [16], we proposed the following general expression, written in terms of the variables (ρ, \mathbf{v}, c, s) , which encompasses the previous nonstandard expressions as special cases:

$$S^a = \int_\Omega \rho s + \frac{\rho^a}{2} \lambda_s \Gamma^2 (\nabla c), \quad (89)$$

$$H^a = \int_\Omega \frac{\rho}{2} |\mathbf{v}|^2 + \rho u(\rho, s, c) + \frac{\rho^a}{2} \lambda_u \Gamma^2 (\nabla c). \quad (90)$$

Upon setting $a = 0$, Eqs. (89) and (90) reduce to the expressions of [31–33], while upon setting $a = 1$ they reduce to those of [34], provided the choice of an isotropic surface energy is assumed, viz., $\Gamma(\nabla c) = |\nabla c|$. These were apparently modeled after the free-energy expression of the Cahn-Hilliard equation which is a linear combination of energy and entropy.

In [16], the entropy of Eq. (89) was simplified to the standard form of Eq. (64) by a coordinate change. This resulted in the more complicated internal energy function of Eq. (68), as compared with Eq. (90), where in the former the σ in the argument of u is replaced by $\sigma = \bar{\sigma} - \frac{\lambda_s}{2} \Gamma^2 (\nabla c)$. Given that an incremental volume of fluid contains both phases, it is perhaps not surprising that the internal energy should reflect this.

In [16] we proceeded with the UT algorithm and obtained a metriplectic 4-bracket for a generalized system which includes both the $a = 0$ and $a = 1$ cases (with a small correction to [34]). However, because the development of Sec. III A was not yet available, step (4) of the algorithm required some investigation on how to appropriately place the following pseudodifferential operator in Σ :

$$\mathcal{L}^{\tilde{c}}(F_{\tilde{c}}) := \nabla(F_{\tilde{c}} + \nabla \cdot (\lambda_s \Gamma \xi F_{\sigma}) / \rho). \quad (91)$$

Given that the operators $\mathcal{L}^{(\alpha)}$ can be placed at will in the expression of Σ of Eq. (50), it is clear that our new development can reproduce and generalize our previous work and produce an even-more general class of thermodynamically consistent models that describe two-phase flows. Instead of pursuing this, we will show in the next section how the development of Sec. IV A produces and generalizes models by Brenner and others.

C. Brenner-Navier-Stokes-Fourier (BNSF)

In a series of papers [36–39], Brenner proposed a modification to address what he believed to be certain limitations of the traditional Navier-Stokes-Fourier system. In this section, we will show that his theory emerges as a special case of our development of Sec. IV A. Moreover, our theory shows the following: how to unambiguously delineate the dissipative dynamics from the nondissipative (Hamiltonian) dynamics; that generalizations of Brenner’s theory by other authors are, again, special cases of our theory; in particular they all emerge from Eq. (51); all these theories amount to modifications of the form of dissipation in the Navier-Stokes equations.

Brenner’s proposed modification is based on a “biveLOCITY theory” which introduces the idea of two distinct velocities: the mass velocity \mathbf{v}_m , which corresponds to the conventional understanding, and a volume velocity denoted by \mathbf{v} . In studies of classical continuum fluid mechanics, these velocities are assumed to be identical. However, Brenner argued that, in general, $\mathbf{v}_m \neq \mathbf{v}$. This hypothesis leads to a nontraditional extension of the NSF system, known as the Brenner-Navier-Stokes-Fourier (BNSF) system, which is formulated as follows:

$$\partial \rho + \nabla \cdot (\rho \mathbf{v}_m) = 0, \quad (92)$$

$$\partial(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v}_m \mathbf{v}) = \nabla \cdot (-p \bar{I} + \bar{\bar{\Lambda}} : \nabla \mathbf{v}), \quad (93)$$

$$\begin{aligned}\partial \sigma + \nabla \cdot (\sigma \mathbf{v}_m) &= \nabla \cdot \left[\frac{\bar{\kappa}}{T} \cdot \nabla T \right. \\ &\quad \left. - \frac{\mathbf{w}}{T} (p + u - \rho \alpha) \right] + \dot{\sigma}^{\text{prod}}.\end{aligned}\quad (94)$$

Here, as before, $u(\rho, s)$ is the internal energy per unit mass, α is a new unconstrained phenomenological parameter, and \mathbf{w} represent the velocity difference vector,

$$\mathbf{w} = \mathbf{v} - \mathbf{v}_m.$$

(Note, in the works of Brenner the symbol \mathbf{J} is used for this velocity difference.)

It remains to close this system by determining \mathbf{w} in terms of the dynamical variables. In [36], Brenner first proposed $\mathbf{w} = \alpha \nabla \ln(\rho)$. Later in [38] and [11,40], using Öttinger’s version of GENERIC, it was settled on the following form for \mathbf{w} :

$$\mathbf{w} = \tilde{D}(\nabla p - \gamma \nabla T), \quad (95)$$

where, for simplicity, we introduced the diffusionlike coefficient $\tilde{D} := D' / (\rho^2 T)$ and the parameter γ is defined by

$$\rho \alpha - u = p - \gamma T.$$

Thus, the system contains one parameter, either α or γ . By taking $\gamma = (\frac{\partial p}{\partial T})_\rho$, Brenner established that the velocity dif-

ference \mathbf{w} becomes

$$\mathbf{w} = \frac{\tilde{D}}{\kappa_T} \nabla \ln \rho, \quad (96)$$

where $\kappa_T = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial p} \right)_T$ is the coefficient of isothermal compressibility, assumed to be non-negative. In these works, it is claimed that this is the most general possible constitutive equation for the velocity difference \mathbf{w} . However, a generalization was given in [41], which we will further generalize below using the UT algorithm.

To view the above BNSF system in a form adapted to the UT algorithm, we interpret \mathbf{v} to be the usual velocity field, and write the system in terms of NSF variables $\xi = (\rho, \mathbf{m} = \rho \mathbf{v}, \sigma)$ as follows:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = \nabla \cdot (\rho \mathbf{w}), \quad (97)$$

$$\partial_t \mathbf{m} + \nabla \cdot (\mathbf{m} \otimes \mathbf{v}) = \nabla \cdot (-\rho \bar{I} + \bar{\bar{\Lambda}} : \nabla \mathbf{v} + \mathbf{m} \otimes \mathbf{w}), \quad (98)$$

$$\partial_t \sigma + \nabla \cdot (\sigma \mathbf{v}) = \nabla \cdot \left[\frac{\bar{\kappa}}{T} \nabla T + (\sigma - \gamma) \mathbf{w} \right] + \dot{\sigma}^{\text{prod}}. \quad (99)$$

Except for γ and \mathbf{w} , the quantities above are defined as for the NSF system. Evidently, from Eqs. (97), (98), and (99), it is seen that the fluxes are given by the following:

$$\mathbf{J}_\rho = -\rho \mathbf{w}, \quad (100)$$

$$\bar{J}_\mathbf{m} = -\bar{\bar{\Lambda}} : \nabla \mathbf{v} - \mathbf{m} \otimes \mathbf{w}, \quad (101)$$

$$\mathbf{J}_s = -\frac{\bar{\kappa}}{T} \cdot \nabla T - (\sigma - \gamma) \mathbf{w}, \quad (102)$$

which determine the phenomenological coefficients in terms of \mathbf{w} .

Given both the above and the results of Sec. IV A, there is no need to run through the steps of the UT algorithm: the variables ξ are the same, the forms of S and H of Eqs. (45) and (46) are the same, the Poisson bracket is again the Morrison-Greene Poisson bracket of Eq. (48) and the form of the operators $\mathcal{L}^{(\alpha)}$ are also the same. Thus, it only remains to determine the phenomenological coefficients and these are provided by matching Eqs. (100), (101), and (102) with Eq. (51).

Comparison of Eq. (100) with the first equation of (51) leads to the determination of \mathbf{w} . We have

$$\mathbf{J}_\rho = -L^{\rho\rho} \cdot \nabla H_\rho - L^{\rho\mathbf{m}} : \nabla H_\mathbf{m} - L^{\rho\sigma} \cdot \nabla H_\sigma, \quad (103)$$

where the 2-tensors $L^{\rho\rho}$ and $L^{\rho\sigma}$ and the 3-tensor $L^{\rho\mathbf{m}}$ are contracted as in Eq. (54). From the functional derivative H_ρ of Eq. (55) and the local thermodynamic identities of Eq. (47), we find

$$\nabla H_\rho = -\frac{\sigma}{\rho} \nabla T + \frac{1}{\rho} \nabla p - (\nabla \mathbf{v}) \cdot \mathbf{v} \quad (104)$$

and

$$\nabla p = \rho \nabla H_\rho + (\nabla H_\mathbf{m}) \cdot \mathbf{m} + \sigma \nabla H_\sigma. \quad (105)$$

Thus, the difference velocity \mathbf{w} of Eq. (95) can be written as the following linear combination of ∇H_ρ , $\nabla H_\mathbf{m}$ and ∇H_σ :

$$\mathbf{w} = \tilde{D} \rho \nabla H_\rho + \tilde{D} (\nabla H_\mathbf{m}) \cdot \mathbf{m} + \tilde{D} \hat{\sigma} \nabla H_\sigma, \quad (106)$$

where we defined $\hat{\sigma} := \sigma - \gamma$. Therefore, according to Eq. (100),

$$\mathbf{J}_\rho = -\tilde{D} \rho^2 \nabla H_\rho - \tilde{D} \rho (\nabla H_\mathbf{m}) \cdot \mathbf{m} - \tilde{D} \rho \hat{\sigma} \nabla H_\sigma, \quad (107)$$

and comparison with Eq. (103) yields

$$L^{\rho\rho} = \tilde{D} \rho^2 \bar{I}, \quad L^{\rho\mathbf{m}} = \tilde{D} \rho \bar{I} \otimes \mathbf{m}, \quad L^{\rho\sigma} = \tilde{D} \rho \hat{\sigma} \bar{I}. \quad (108)$$

Similarly, using Eqs. (51), (101), and (106),

$$\begin{aligned} \bar{J}_\mathbf{m} &= -L^{\mathbf{m}\rho} \otimes \nabla H_\rho - L^{\mathbf{m}\mathbf{m}} : \nabla H_\mathbf{m} - L^{\mathbf{m}\sigma} \otimes \nabla H_\sigma \\ &= -\bar{\bar{\Lambda}} : \nabla H_\mathbf{m} - \mathbf{m} \otimes \\ &\quad (\tilde{D} \rho \nabla H_\rho + \tilde{D} (\nabla H_\mathbf{m}) \cdot \mathbf{m} + \tilde{D} \hat{\sigma} \nabla H_\sigma), \end{aligned} \quad (109)$$

whence we see

$$\begin{aligned} L^{\mathbf{m}\rho} &= \tilde{D} \rho \mathbf{m}, \quad L^{\mathbf{m}\sigma} = \tilde{D} \hat{\sigma} \mathbf{m}, \quad \text{and} \\ L^{\mathbf{m}\mathbf{m}} &= \bar{\bar{\Lambda}} + \tilde{D} \mathbf{m} \otimes \bar{I} \otimes \mathbf{m}. \end{aligned} \quad (110)$$

Note, using our convention $(\bar{\bar{\Lambda}} : \nabla \mathbf{v})_{ij} = \Lambda_{ijkl} \partial_k v_l$ we have

$$\begin{aligned} (\mathbf{m} \otimes \bar{I} \otimes \mathbf{m}) : \nabla H_\mathbf{m} &_{ij} = (m_i \delta_{jk} m_l) \partial_k v_l \\ &= m_i m_l \partial_j v_l. \end{aligned} \quad (111)$$

Finally, using Eqs. (51), (102), and (106),

$$\begin{aligned} \mathbf{J}_s &= -L^{\sigma\rho} \cdot \nabla H_\rho - L^{\sigma\mathbf{m}} : \nabla H_\mathbf{m} - L^{\sigma\sigma} \cdot \nabla H_\sigma \\ &= -\frac{\bar{\kappa}}{T} \cdot \nabla H_\sigma \\ &\quad - \hat{\sigma} (\tilde{D} \rho \nabla H_\rho + \tilde{D} (\nabla H_\mathbf{m}) \cdot \mathbf{m} + \tilde{D} \hat{\sigma} \nabla H_\sigma); \end{aligned} \quad (112)$$

whence we see

$$L^{\sigma\rho} = \tilde{D} \rho \hat{\sigma} \bar{I}, \quad L^{\sigma\sigma} = \frac{\bar{\kappa}}{T} + \tilde{D} \hat{\sigma}^2 \bar{I} \quad (113)$$

$$L^{\sigma\mathbf{m}} = \tilde{D} \hat{\sigma} \bar{I} \otimes \mathbf{m}. \quad (114)$$

With these phenomenological coefficients, we obtain directly the operators M and Σ . Again, M is chosen, as in Eq. (49), while Σ is given as follows:

$$\begin{aligned} \Sigma(dF, dG) &= \frac{1}{T} \left[\tilde{D} \rho^2 \nabla F_\rho \cdot \nabla G_\rho \right. \\ &\quad + \tilde{D} \rho (\nabla F_\rho \cdot (\nabla G_\mathbf{m}) \cdot \mathbf{m} + \nabla G_\rho \cdot (\nabla F_\mathbf{m}) \cdot \mathbf{m}) \\ &\quad + \tilde{D} \rho \hat{\sigma} (\nabla F_\rho \cdot \nabla G_\sigma + \nabla G_\rho \cdot \nabla F_\sigma) \\ &\quad + \nabla F_\mathbf{m} : (\bar{\bar{\Lambda}} + \tilde{D} \mathbf{m} \otimes \bar{I} \otimes \mathbf{m}) : \nabla G_\mathbf{m} \\ &\quad + \tilde{D} \hat{\sigma} (\nabla F_\sigma \cdot (\nabla G_\mathbf{m}) \cdot \mathbf{m} + \nabla G_\sigma \cdot (\nabla F_\mathbf{m}) \cdot \mathbf{m}) \\ &\quad \left. + \nabla F_\sigma \cdot \left(\frac{\bar{\kappa}}{T} + \tilde{D} \hat{\sigma}^2 \bar{I} \right) \cdot \nabla G_\sigma \right]. \end{aligned} \quad (115)$$

Note, in the penultimate line of Eq. (115) we have used

$$\nabla F_\sigma \cdot \bar{I} \otimes \mathbf{m} : \nabla G_\mathbf{m} = \nabla F_\sigma \cdot (\nabla G_\mathbf{m}) \cdot \mathbf{m}. \quad (116)$$

[Recall Eq. (54).] The metriplectic 4-bracket $(., .; ., .)$ that comes from the K-N product of M and Σ is the following:

$$\begin{aligned}
 (F, K; G, N) = & \int_{\Omega} \frac{K_{\sigma} N_{\sigma}}{T} \left[\tilde{D} \rho^2 \nabla F_{\rho} \cdot \nabla G_{\rho} + \tilde{D} \rho (\nabla F_{\rho} \cdot (\nabla G_{\mathbf{m}}) \cdot \mathbf{m} + \nabla G_{\rho} \cdot (\nabla F_{\mathbf{m}}) \cdot \mathbf{m}) \right. \\
 & + \tilde{D} \rho \hat{\sigma} (\nabla F_{\rho} \cdot \nabla G_{\sigma} + \nabla G_{\rho} \cdot \nabla F_{\sigma}) + \nabla F_{\mathbf{m}} : (\bar{\bar{\Lambda}} + \tilde{D} \mathbf{m} \otimes \bar{I} \otimes \mathbf{m}) : \nabla G_{\mathbf{m}} \\
 & + \tilde{D} \hat{\sigma} (\nabla F_{\sigma} \cdot (\nabla G_{\mathbf{m}}) \cdot \mathbf{m} + \nabla G_{\sigma} \cdot (\nabla F_{\mathbf{m}}) \cdot \mathbf{m}) + \nabla F_{\sigma} \cdot \left(\frac{\bar{\kappa}}{T} + \tilde{D} \hat{\sigma}^2 \bar{I} \right) \cdot \nabla G_{\sigma} \left. \vphantom{\int_{\Omega}} \right] \\
 & - \frac{K_{\sigma} G_{\sigma}}{T} \left[\tilde{D} \rho^2 \nabla F_{\rho} \cdot \nabla N_{\rho} + \tilde{D} \rho (\nabla F_{\rho} \cdot (\nabla N_{\mathbf{m}}) \cdot \mathbf{m} + \nabla N_{\rho} \cdot (\nabla F_{\mathbf{m}}) \cdot \mathbf{m}) \right. \\
 & + \tilde{D} \rho \hat{\sigma} (\nabla F_{\rho} \cdot \nabla N_{\sigma} + \nabla N_{\rho} \cdot \nabla F_{\sigma}) + \nabla F_{\mathbf{m}} : (\bar{\bar{\Lambda}} + \tilde{D} \mathbf{m} \otimes \bar{I} \otimes \mathbf{m}) : \nabla N_{\mathbf{m}} \\
 & + \tilde{D} \hat{\sigma} (\nabla F_{\sigma} \cdot (\nabla N_{\mathbf{m}}) \cdot \mathbf{m} + \nabla N_{\sigma} \cdot (\nabla F_{\mathbf{m}}) \cdot \mathbf{m}) + \nabla F_{\sigma} \cdot \left(\frac{\bar{\kappa}}{T} + \tilde{D} \hat{\sigma}^2 \bar{I} \right) \cdot \nabla N_{\sigma} \left. \vphantom{\int_{\Omega}} \right] \\
 & + \frac{F_{\sigma} G_{\sigma}}{T} \left[\tilde{D} \rho^2 \nabla K_{\rho} \cdot \nabla N_{\rho} + \tilde{D} \rho (\nabla K_{\rho} \cdot (\nabla N_{\mathbf{m}}) \cdot \mathbf{m} + \nabla N_{\rho} \cdot (\nabla K_{\mathbf{m}}) \cdot \mathbf{m}) \right. \\
 & + \tilde{D} \rho \hat{\sigma} (\nabla K_{\rho} \cdot \nabla N_{\sigma} + \nabla N_{\rho} \cdot \nabla K_{\sigma}) + \nabla K_{\mathbf{m}} : (\bar{\bar{\Lambda}} + \tilde{D} \mathbf{m} \otimes \bar{I} \otimes \mathbf{m}) : \nabla N_{\mathbf{m}} \\
 & + \tilde{D} \hat{\sigma} (\nabla K_{\sigma} \cdot (\nabla N_{\mathbf{m}}) \cdot \mathbf{m} + \nabla N_{\sigma} \cdot (\nabla K_{\mathbf{m}}) \cdot \mathbf{m}) + \nabla K_{\sigma} \cdot \left(\frac{\bar{\kappa}}{T} + \tilde{D} \hat{\sigma}^2 \bar{I} \right) \cdot \nabla N_{\sigma} \left. \vphantom{\int_{\Omega}} \right] \\
 & - \frac{F_{\sigma} N_{\sigma}}{T} \left[\tilde{D} \rho^2 \nabla K_{\rho} \cdot \nabla G_{\rho} + \tilde{D} \rho (\nabla K_{\rho} \cdot (\nabla G_{\mathbf{m}}) \cdot \mathbf{m} + \nabla G_{\rho} \cdot (\nabla K_{\mathbf{m}}) \cdot \mathbf{m}) \right. \\
 & + \tilde{D} \rho \hat{\sigma} (\nabla K_{\rho} \cdot \nabla G_{\sigma} + \nabla G_{\rho} \cdot \nabla K_{\sigma}) + \nabla K_{\mathbf{m}} : (\bar{\bar{\Lambda}} + \tilde{D} \mathbf{m} \otimes \bar{I} \otimes \mathbf{m}) : \nabla G_{\mathbf{m}} \\
 & + \tilde{D} \hat{\sigma} (\nabla K_{\sigma} \cdot (\nabla G_{\mathbf{m}}) \cdot \mathbf{m} + \nabla G_{\sigma} \cdot (\nabla K_{\mathbf{m}}) \cdot \mathbf{m}) + \nabla K_{\sigma} \cdot \left(\frac{\bar{\kappa}}{T} + \tilde{D} \hat{\sigma}^2 \bar{I} \right) \cdot \nabla G_{\sigma} \left. \vphantom{\int_{\Omega}} \right]. \quad (117)
 \end{aligned}$$

Upon insertion of S as given by Eq. (45) and H as given by Eq. (46), the system of (97), (98), and (99) is produced according to

$$\begin{aligned}
 \partial_t \rho &= \{\rho, H\} + (\rho, H; S, H), \\
 \partial_t \mathbf{m} &= \{\mathbf{m}, H\} + (\mathbf{m}, H; S, H), \\
 \partial_t \sigma &= \{\sigma, H\} + (\sigma, H; S, H),
 \end{aligned}$$

and the total entropy production is governed by the following:

$$\begin{aligned}
 \dot{S} &= (S, H; ., S, H) = \int_{\Omega} \Sigma(dH, dH) \\
 &= \int_{\Omega} \frac{1}{\tilde{D} T} \mathbf{w} \cdot \mathbf{w} + \nabla T \cdot \frac{\bar{\kappa}}{T} \cdot \nabla T + \nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v} \\
 &= \int_{\Omega} \frac{1}{T} \left[\tilde{D} |\mathbf{v}_m - \mathbf{v}|^2 + \nabla T \cdot \frac{\bar{\kappa}}{T} \cdot \nabla T \right. \\
 &\quad \left. + \nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v} \right] \geq 0. \quad (118)
 \end{aligned}$$

Alternatively, using Eq. (96):

$$\begin{aligned}
 \dot{S} &= \int_{\Omega} \frac{1}{T} \left[\frac{\tilde{D}}{\kappa_T^2 \rho^2} |\nabla \rho|^2 + \nabla T \cdot \frac{\bar{\kappa}}{T} \cdot \nabla T \right. \\
 &\quad \left. + \nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v} \right] \geq 0. \quad (119)
 \end{aligned}$$

Therefore, we shown that the system proposed by Brenner [38] can be understood as an extension of the classical Navier-Stokes-Fourier, achieved by introducing an additional dissipation mechanism. Brenner postulates that his hypothesis primarily alters the ideal part of the dynamics. However, if by ideal is meant Hamiltonian, we see that this is not true, since the Hamiltonian part is still governed by the Poisson bracket of [22]. In addition, Brenner links this modification to the compressibility of the fluid and suggests that the mass velocity \mathbf{v}_m and volume velocity \mathbf{v} coincide if, and only if, the fluid is incompressible (i.e., $\rho = \text{const}$).

We have also shown that the expression of \mathbf{w} given by Eq. (95) is not the most general form giving a thermodynamically consistent system; from Eq. (103)

$$\mathbf{w} = (L^{\rho\rho} \cdot \nabla H_{\rho} + L^{\rho\mathbf{m}} : \nabla H_{\mathbf{m}} + L^{\rho\sigma} \cdot \nabla H_{\sigma}) / \rho, \quad (120)$$

whence we see that \mathbf{w} can be any linear combination of ∇H_{ρ} , $\nabla H_{\mathbf{m}}$ and ∇H_{σ} contracted appropriately with the 2-tensors $L^{\rho\rho}$ and $L^{\rho\sigma}$ and the 3-tensor $L^{\rho\mathbf{m}}$. Insertion of the expression for \mathbf{w} of Eq. (120), with the Hamiltonian of your choice, into Eq. (94) gives a thermodynamically consistent generalizations of the BNSF.

In a more recent paper [41], thermodynamically consistent generalizations of the BNSF system were given. In concluding this section, we show that the various generalizations of this

reference are again special cases of our metriplectic system of Sec. IV A with Eq. (120). Specifically, the cases of [41] (rewritten in our notation) are as follows.

Equation (77) of [41]:

$$\mathbf{w} = \kappa_m \nabla \ln \rho, \quad (121)$$

where $\kappa_m = \tilde{D}/\kappa_T$, is Brenner's (96) using $\gamma = (\frac{\partial p}{\partial T})_\rho$.

Equation (78) of [41]:

$$\mathbf{w} = \kappa_T \nabla \ln T = \frac{\kappa_T}{T} \nabla H_\sigma, \quad (122)$$

is given by our Eq. (120) with the choices

$$L^{\rho\rho} = L^{\rho\mathbf{m}} = 0, \quad L^{\rho\sigma} = \rho \frac{\kappa_T}{T} \bar{I} \quad (123)$$

Equation (79) of [41]:

$$\mathbf{w} = \kappa_p \nabla \ln p = \frac{\kappa_p}{p} \nabla p, \quad (124)$$

which is produced in our formalism as

$$\mathbf{w} = \frac{\kappa_p}{p} (\rho \nabla H_\rho + (\nabla H_{\mathbf{m}}) \cdot \mathbf{m} + \sigma \nabla H_\sigma), \quad (125)$$

where κ_p is the thermal conductivity at constant pressure and the third equality follows from Eq. (105). Equation (124) is given by our Eq. (120) with the choices

$$\begin{aligned} L^{\rho\rho} &= \rho^2 \frac{\kappa_p}{p} \bar{I}, & L^{\rho\mathbf{m}} &= \rho \kappa_p \bar{I} \otimes \mathbf{m}; \\ L^{\rho\sigma} &= \rho \kappa_p \sigma \bar{I}. \end{aligned} \quad (126)$$

Equation (80) of [41]:

$$\mathbf{w} = \kappa_\tau \nabla \times \mathbf{v} = \kappa_\tau \nabla \times H_{\mathbf{m}}, \quad (127)$$

where κ_τ is another phenomenological quantity. Equation (127) is a particular case of our theory by taking

$$L^{\rho\rho} = 0, \quad L^{\rho\mathbf{m}} = \rho \kappa_\tau \boldsymbol{\epsilon}, \quad L^{\rho\sigma} = 0, \quad (128)$$

where $\boldsymbol{\epsilon}$ is the Levi-Civita 3-tensor (density) and contraction is defined by Eq. (54). Note, the tensorial inconsistency of Eq. (127) can be resolved by assuming κ_τ is a pseudoscalar.

V. CONCLUSION

The main contribution of this paper is the unified thermodynamical algorithm that uses the metriplectic 4-bracket of previous work [10,16,18] to methodically lead one to general classes of thermodynamically consistent systems. An important and novel by-product of this algorithm is the definition of fluxes given by (2). In Sec. II we reviewed the Hamiltonian and 4-bracket frameworks, on which the UT algorithm is based. This is followed by Sec. III that contains the main new contribution: the unambiguous determination of the metriplectic 4-bracket. In Sec. IV we present examples that generalize previous results. In particular, we showed that the Brenner-Navier-Stokes-Fourier system and its generalizations of [41] are special cases of our generalization of the Navier-Stokes-Fourier system. They all amount to modifying the dissipation in the Navier-Stokes equations.

The dichotomies of dissipative vs nondissipative and reversible vs irreversible can be confused or used inappropriately, particularly when one is dealing with systems that contain a set of conservation laws, such as those of Eq. (27). One clear distinction can be made: that between Hamiltonian vs non-Hamiltonian, where the former is an unambiguous definition of what is meant by nondissipative. The distinction between reversible and irreversible is also often confused. All systems of autonomous ordinary differential equations are reversible because the solution is a one-parameter Lie group, and not all Hamiltonian systems have time reversible symmetry, a special case of a point symmetry. Again, there is no confusion if one distinguishes Hamiltonian from nonHamiltonian, and the metriplectic 4-bracket formalism makes it clear which parts are Hamiltonian and which parts are dissipative.

Another dichotomy concerns the placement of temperature in the metriplectic formalism. Temperature may appear as a result of the assumption of local thermodynamic equilibrium, e.g., via an internal energy function u in the Hamiltonian, or it may appear in the assumed forms of the phenomenological coefficients $L^{\alpha\beta}$. In the first work on the metriplectic dynamics of the NSF fluid [2], it was observed that the temperature needed to be placed in an ad hoc manner so as to make things work out. Similarly, the same observation was noted in Chap. 3 of [11]. A resolution of this dichotomy is achieved with the UT algorithm, where temperature may appear according to Eqs. (27) and (39), or in the choice of phenomenological coefficients. It is interesting to note that once M and Σ are chosen and the 4-bracket is determined, one can use any Hamiltonian and obtain a thermodynamically consistent system. This provides additional freedom for modeling.

In closing we mention some possibilities for future work. The results of this paper pertain to macroscopic or purely continuum theories. Underlying kinetic theory can place constraints on such continuum theories. For example, in [42] it was noted that the results of Brenner are in disagreement with a number of kinetic-theory studies. In the present context, an open question is how to connect the 4-bracket to a class of underlying kinetic theories with dissipative mechanisms, such as collision operators. On the kinetic level, a metriplectic 4-bracket was given in [18] for a generalization of the Landau collision operator and the same can be done for a variety of kinetic theories. So far, no connection has been made between fluid and kinetic 4-brackets.

The UT algorithm can be both restricted and generalized. For example, additional symmetries beyond Onsager, such as Galilean or Poincaré invariance, can constrain the choices of M and Σ . These symmetries might be traced from a kinetic theory or considered on the macroscopic level. Here we have not considered these possibilities, so as to keep the development general. An avenue for further generalization would be to break the linear force-flux relations of Eqs. (1) or (2). The essential feature of thermodynamic consistency is global asymptotic stability and the concomitant production of entropy. Dynamical systems with global asymptotic stability can be recast into the form of Eqs. (1) or (2) by using rectification arguments similar to those described in [10]. Rectification arguments fail when additional fixed points exist. Systems with this property would not be expected to be

thermodynamically consistent, but one could still linearize within basins of attraction.

Lastly, we mention that the metriplectic 4-bracket can be used to obtain thermodynamically consistent numerical algorithms for fluid and plasma systems. Previously, 2-brackets have been used and proposed in [43–47] to obtain thermodynamically consistent numerics, i.e., where the semi-discrete equations are a finite-dimensional metriplectic system in terms of the 2-bracket. However, recently in [29], the 4-bracket was found to be particularly useful because maintaining symmetries while projecting onto a Galerkin basis is, essentially, automatic.

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DATA AVAILABILITY

No data were created or analyzed in this study.

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