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Two-Phase Fluid Dynamics: Modeling, Metriplectic Formalism, and Well-Posedness Analysis

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Abstract

Cahn-Hilliard-Navier-Stokes (CHNS) systems describe two-phase flows, such as liquids containing bubbles. Obtaining constitutive relations for general dissipative processes in such systems that remain thermodynamically consistent is challenging. We demonstrate how the metriplectic 4-bracket formalism provides a straightforward, algorithmic approach to this problem. This approach, called the unified thermodynamic algorithm (UTA), constructs thermodynamically consistent dynamical systems combining Hamiltonian and dissipative parts that conserve energy while producing entropy. A key feature of the UTA is the force-flux relation $\mathbf{J}^\alpha = -L^{\alpha\beta}\nabla(\delta H/\delta\xi^\beta)$, where $L^{\alpha\beta}$ are phenomenological coefficients, H is the Hamiltonian, and ξ^β are dynamical variables. The algorithm is applied to various systems, including Navier-Stokes-Fourier and Brenner-Navier-Stokes-Fourier models, with significant generalizations obtained for CHNS systems. We exploit the underlying mathematical structures to ensure thermodynamic consistency is preserved during discretization of fluid models. This relies on (1) maintaining the symmetries and degeneracies of the Poisson and metriplectic 4-brackets in spatial semi-discretizations and (2) employing energy-conserving time-stepping schemes. A minimally simple yet nontrivial example— one-dimensional thermal-fluid model—is treated, showing that preserving these properties in Galerkin spatial discretizations is relatively straightforward. This suggests a pathway toward thermodynamically consistent discretizations of more complex fluid models using specialized Galerkin methods. Furthermore, we investigate the well-posedness of the anisotropic, incompressible CHNS system with variable density in a bounded smooth domain $\Omega \subset \mathbb{R}^d$. This extends previous isotropic studies by incorporating anisotropic surface energy, represented by $\mathfrak{F} = \int_\Omega \frac{\epsilon}{2}\Gamma^2(\nabla\phi)$. Using a Galerkin approximation scheme, we prove the existence of global weak solutions in two and three dimensions ($d = 2, 3$). A crucial step in extending the existence of approximate solutions from local to global is the use of Bihari's inequality combined with a fixed-point argument.

The main body of this thesis consists of the following publications, submitted papers and scientific meetings:

Publications and Submitted papers

1. A. Zaidni, P J. Morrison, "Metriplectic 4-bracket algorithm for constructing thermodynamically consistent dynamical systems," *Physical Review E*, `https://link.aps.org/doi/10.1103/r2lb-xkq6`, 2025 (Accepted).

2. W. Barham, P J. Morrison, A. Zaidni, "A thermodynamically consistent discretization of 1D thermal-fluid models using their metriplectic 4-bracket structure," *Communications in Nonlinear Science and Numerical Simulation*, 108683, 2025.

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3. A. Zaidni, P J. Morrison, S. Benjelloun,"Thermodynamically consistent Cahn-Hilliard-Navier-Stokes equations using the metriplectic dynamics formalism," *Physica D: Nonlinear Phenomena*, 468, 134303, 2024.

4. A. Zaidni, S. Benjelloun, R. Boukharfane "Global existence of weak solutions to incompressible anisotropic Cahn-Hilliard-Navier-Stokes system ", *arXiv preprint arXiv:2412.05757, submitted*, 2025.

5. S. Benjelloun, A. Zaidni "On sound dispersion and attenuation in simple and multi-fluids due to thermal and viscous effects", *Proceedings of Meetings on Acoustics*, 45, 1, 2021.

Scientific Meetings

1. A. Zaidni, P J. Morrison, S. Benjelloun, "On ideal and real two-fluid mixtures of dispersed type: bubbly and droplet flow," *77th Annual Meeting of the Division of Fluid Dynamics (APS), November 24–26, 2024; Salt Lake City, Utah.*

2. A. Zaidni, P J. Morrison, S. Benjelloun, "Thermodynamically consistent Cahn-Hilliard Navier-Stokes equations using the metriplectic dynamics formalism," *76th Annual Meeting of the Division of Fluid Dynamics (APS), November 19–21, 2023; Washington, DC.*

3. A. Zaidni, S. Benjelloun, "On sound dispersion and attenuation in simple and multi-fluids due to thermal and viscous effects", *181st Meeting of the Acoustical Society of America, 29 November–3 December 2021, Seattle, Washington*

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INTRODUCTION 1

Two-phase flow refers to the movement of two different types of substances or phases at the same time in a system. These phases can be solid, liquid, or gas. A common example is when a liquid and a gas move together through a pipe, such as steam and water inside a power plant system. Sometimes, the two phases are parts of the same substance, like water and its vapor (steam). In other cases, they can be two different materials, like air and oil, or water and sand. In many industries, two-phase flow happens naturally and is a key part of how machines or systems work. It can be found in chemical plants, oil and gas pipelines, refrigeration systems, power generation (especially in boilers and condensers), and even in natural settings like oceans and underground reservoirs. This type of flow plays a big role in processes involving heating, cooling, or mixing materials. One of the most studied and used types of two-phase flow is liquid-gas flow, especially when a change of phase occurs, like boiling or condensation. This is important because phase change involves a lot of heat transfer, which can be used to control temperature or energy inside a system. Engineers and researchers pay close attention to how heat and pressure behave in these situations, as they affect how safe and efficient a system is.

Understanding two-phase flow is challenging due to the fact that the two phases typically move at different velocities and possess distinct thermodynamic properties. For example, the gas may move faster than the liquid, or one may heat up or cool down faster. In some cases, the boundary between the two phases can be clearly seen, like oil floating on water. In other cases, such as bubbles in boiling water, the boundary changes constantly and is hard to track. To describe and predict two-phase flow, scientists use models. There are mainly two types of models: the separated flow model and the homogeneous flow model. In the separated flow model, each

phase is treated as if it flows separately, each with its own speed and thermodynamic proprieties. In contrast, the homogeneous flow model assumes both phases move and behave in the same way. Each model is used depending on how the phases interact and how complex the situation is. Engineers use data from two-phase flow studies to make systems safer and more reliable. For example, in pipelines, knowing how gas and liquid interact helps prevent accidents like pipe bursts or pressure build-up. In heat exchangers, predicting how fluids change phases can improve energy efficiency. If these flows are not well understood or controlled, they can lead to problems like corrosion, erosion, or equipment failure.

Overall, two-phase flow is a complex but important topic in fluid mechanics and engineering. It requires careful analysis and good understanding of both the physical properties of the fluids and the way they move. With proper models and tools, it is possible to design systems that work efficiently and safely even when multiple phases are involved. The well-known Navier-Stokes equations govern the motion of a single-phase fluid. However, in the case of two-phase fluids, chemical reactions, changes of phase, and migration between substances of phases become significant and cannot be disregarded. J. W. Cahn and J. E. Hilliard were the first to formulate the mathematical equations that describe phase separation in a such a binary fluid [Cahn and Hilliard, 1958]. Here we investigate generalizations that combine the Cahn-Hilliard equation with equations that describe the dynamics of fluid flow, referred to as Cahn-Hilliard-Navier-Stokes (CHNS) systems. CHNS systems aim to describe the hydrodynamic properties of a mixture of two phases such as bubbles in a liquid. To narrow down the already broad scope, we assume that the two fluids share the same velocity field, yet we allow for both extended thermodynamics and diffusive interfaces between the two phases.

A substantial hurdle in developing CHNS type systems, systems with a variety of constitutive relations, is to ensure thermodynamic consistency, i.e., adherence to the first law of thermodynamics, which in this context is to produce a set of dynamical equations that conserve energy, and the second law which in this context means the dynamical production of entropy, ensuring the relaxation (asymptotic stability) to thermodynamic equilibrium. Here, we propose an algorithm for constructing such systems, an algorithm that produces a large set of CHNS systems.

A central challenge in modeling general dynamical systems, particularly in fluid dynamics, is ensuring thermodynamic consistency—namely, satisfying the first law (energy conservation) and the second law (entropy production). In this thesis, we develop a systematic procedure for constructing such systems in infinite-dimensional settings. The approach is based on the metriplectic formalism, a nonclassical frame-

work that naturally incorporates both Hamiltonian (reversible) and dissipative (irreversible) dynamics. The resulting systems, especially in the context of two-phase fluid flow, exhibit the correct thermodynamic structure. Moreover, the framework extends to the discrete level, allowing the design of numerical schemes that retain thermodynamic consistency. Under suitable assumptions, we also investigate the well-posedness of the resulting two-phase models using tools from functional analysis.

The contributions of this thesis are organized into five chapters. The chapter 2 is structured as follows: We provide an overview of the metriplectic framework, where foundational concepts are reviewed, starting with the Hamiltonian formalism (Sec. 2.1) and moving to the metriplectic formalism (Sec. 2.2). Therefor, we linked the metriplectic 4-bracket to the original binary metriplectic formalism (Metriplectic 2-bracket) (Sec. 2.3). 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. 2.4, we focus on the derivation of the metriplectic 4-bracket. Here, a systematic approach to the theory is developed (Sec. 2.4), followed by a discussion on the relationship to non-equilibrium thermodynamics principles (Sec. 2.4.1).

In chapter 3, we propose the Metriplectic 4-bracket algorithm for constructing thermodynamically consistent dynamical systems in infinite-dimensional. We refer to this algorithm as "Unified thermodynamic algorithm" (UTA). The algorithm has four steps: i) Select a set of dynamical variables. For example in Navier-Stokes-Fourier (NSF) system these will be $\psi \coloneqq \{\mathbf{m} = \rho\mathbf{v}, \rho, \sigma = \rho s\}$, which are the momentum density, mass density, and entropy density, respectively. And for CHNS system $\psi \coloneqq \{\mathbf{m} = \rho\mathbf{v}, \rho, \tilde{c} = \rho c, \sigma = \rho s\}$, which c is the volume concentration of one of the constituents. ii) The next step is to select energy and entropy functionals, H and S, dependent on the dynamical variables. The choice of these functionals is based on the physics of the phenomena one wishes to describe. iii) The third step of the algorithm is to obtain the noncanonical Poisson bracket [see Morrison, 1998b] of the ideal (nondissipative) part of the theory that has the chosen entropy as a Casimir invariant. Since the work of Morrison and Greene [1980], Poisson brackets for a great many systems, including fluid and magnetofluid systems, have been found [e.g. Morrison, 1982, Thiffeault and Morrison, 2000, Abdelhamid et al., 2015, D'Avignon et al., 2016, Zaidni et al., 2023]. Thus, this step may be immediate. Alternatively, it may be achieved by a coordinate change from a known Hamiltonian theory in order to align with the chosen entropy functional. In either case, we obtain at this stage a noncanonical Hamiltonian system. iv) The final step is to construct a metriplectic 4-bracket as described in Morrison and Updike [2023]. Although there

are standard metriplectic 4-bracket constructions, there is freedom at this last step to describe a variety of types of dissipation. However, a natural choice follows upon consideration of the form of an early metriplectic bracket [Morrison, 1984a]. Given H, S, and the 4-bracket, the dynamical system with thermodynamically consistent dissipation is produced.

In this chapter, we present three examples to illustrate the application of the developed theory by applying the UTA. Specifically, the Navier-Stokes-Fourier (NSF) system (Sec. 3.1), and the Brenner-Navier-Stokes-Fourier (BNSF) system (Sec. 3.2) 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.

For two-phase fluid dynamics, we provide a more detailed modeling approach. We apply the algorithm to two cases. First, in Sec. 3.3, we consider a system where the fluid thermodynamics is extended by allowing the internal energy to depend on a concentration variable, with the chemical potential being its thermodynamic dual. Because Gibbs introduced the notion of chemical potential, we refer to the Hamiltonian version of this fluid systems as the Gibbs-Euler (GE) system and the dissipative version as the Gibbs-Navier-Stokes (GNS) system. It is a thermodynamically consistent version of the compressible Navier-Stokes equations with the inclusion of this concentration variable for describing a second phase of the fluid. The GNS system generalizes the early work of Eckart [1940a,b] and the treatment in [de Groot and Mazur, 1962]; it allows for all possible thermodynamics fluxes. Next, in Sec. 3.4, a general form of CHNS system is produced, a form that models surface tension effects and allows for diffuse interfaces. Our work is motivated in large part by the substantial works of Anderson et al. [2000] and Guo and Lin [2015], which we generalize by obtaining a class of systems that includes theirs as special cases. There is a huge literature on this topic and these papers contain many important references to previous work. [Also, see ten Eikelder et al., 2023, for a recent review.]

The GNS system of Sec. 3.3 serves as a straightforward example of our algorithm. In Sec. 3.3.1 we describe the set of dynamical variables, properties of the system, the energy and entropy functionals H and S. This amounts to the first and second steps of the algorithm. Then in Sec. 3.3.2 the Hamiltonian formulation of the dissipation free part of the system is presented. This is the third step of the algorithm where the Poisson bracket is obtained, after a brief review of the noncanonical Hamiltonian formalism. Given the early work of Morrison and Greene [1980] and the classification of extensions in [Thiffeault and Morrison, 2000], this step is immediate. Based on the early and recent works [Morrison, 1984a, Morrison and Updike, 2023] the fourth step

of the algorithm is also immediate. Thus, the thermodynamically consistent GNS system is determined. In Sec. 3.3.4 we obtain the metriplectic 2-bracket equations of motion, and the determined fluxes and affinities, making connection to standard irreversible thermodynamics. Using the results of Sec. 3.3, we proceed in Sec. 3.4 to obtain the main result of the paper, our general CHNS system that can describe diffuse interface effects. The first and second steps of our algorithm are taken in Sec. 3.4.1, while the third step, obtaining the correct Poisson bracket, is undertaken in Sec. 3.4.2. In order to complete this step, one must find the Poisson bracket for which the entropy of the second step is a Casimir invariant, which we find can be achieved by a simple coordinate transformation. The fourth step of the algorithm is taken in Sec. 3.4.3. Here a choice of metriplectic 4-bracket gives a general class of thermodynamically consistent CHNS systems, a class that contains previous results as special cases. The formalism also shows how one can transform to a simple entropy variable at the expense of a more complicated internal energy. We end by giving a simple alternative for modeling the CHNS system (Sec. 3.5). Following in Sec 3.6 by a discussion.

In Chapter 4, we develop a fully discrete, thermodynamically consistent scheme for the one-dimensional Navier–Stokes–Fourier (NSF) model within the metriplectic framework. The spatial discretization is derived from the weak form implied by the metriplectic 4-bracket structure (see Sec. 4.3). For time integration, we initially consider the implicit midpoint method (Sec.4.3.1); however, its failure to conserve total energy motivates the adoption of a discrete gradient method [Quispel and McLaren, 2008, Hairer, 2010], which guarantees energy conservation while preserving the entropy production structure. As a result, the fully discrete system inherits the thermodynamic consistency of the continuous model. In Sec.4.4, we present numerical experiments for the discrete NSF model, tracking the evolution of density, momentum, and entropy. To verify thermodynamic fidelity, we monitor the relative errors in total energy, entropy, and mass, demonstrating that the scheme accurately respects the thermodynamic consistency at the discrete level.

In chapter 5, under some assumption, we study the well-posedness of the anisotropic, incompressible Cahn-Hilliard-Navier-Stokes system with variable density in a bounded smooth domain $\Omega \subset \mathbb{R}^d$ obtained in the chapter 3. This work extends previous studies on the isotropic case [Giorgini and Temam, 2020, Abels et al., 2024, Munteanu, 2024, Rui et al., 2024, Abels et al., 2013] by incorporating anisotropic surface energy. Using a Galerkin approximation scheme, we prove the existence of global weak solutions in both two and three dimensions ($d = 2, 3$).

The final chapter 6 addresses the problem of two-velocity models. Starting from

Hamilton's principle, we derive an ideal two-phase fluid model in Lagrangian form. This description, yields to build principally two different models, The two velocity model (TVM) and the one velocity model which referred to as zero drift velocity model (zDVM). This chapter is structured as follows: The Sec. 6.2 is dedicated to the TVM. We begin by further elucidating the tools needed for the Lagrangian variable description. The equations of motion in the Lagrangian form follow from Hamilton's principle (principal of least action) [see e.g. Morrison, 1998a] which leads us to their Hamiltonian form. Then equations of motion in Lagrangian coordinate are given and mapped to Eulerian coordinate. The Sec. 6.3 is dedicated to the one velocity fluid zDVM model. By including the effect of viscosity on each phase of the fluid and we study the behavior of linear sound waves in this type of (real multi-fluid) medium. This is a classical physics question that is an extension of the wave studies of Kirchhoff [1868] and Stokes [1845] in an ordinary fluid.

CHAPTER

OVERVIEW ON METRIPLECTIC FRAMEWORK 2

2.1 HAMILTONIAN FORMALISM

Let us recall the Hamiltonian formalism in infinite-dimensions. To describe a dynamic one must select 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 the general, we consider the dynamics of classical field theories involving multi-component fields

$$\boldsymbol{\xi}(\mathbf{z},t) = \big(\xi^1(\mathbf{z},t), \xi^2(\mathbf{z},t), \ldots, \xi^N(\mathbf{z},t)\big) \tag{2.1}$$

defined on $\mathbf{z} = (z^1, z^2, \ldots, z^n) \in \Omega$ 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 3-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 $\xi^1, \ldots, \xi^N$ 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 $\boldsymbol{\xi} = (\xi^1, \ldots, \xi^N)$ and observables are functionals that map $\boldsymbol{\xi} \mapsto \mathbb{R}$ at each fixed time. We will denote the space of such functionals by $\mathcal{B}$.

Then a Poisson bracket is an antisymmetric bilinear operator

$$\{\,\cdot\,,\,\cdot\,\}\colon \mathcal{B}\times\mathcal{B}\to\mathcal{B}\,, \tag{2.2}$$

where this bracket is assumed to satisfy the following identities/properties:
(i) Anticommutativity:

$$\{F,G\} = -\{G,F\} \tag{2.3}$$

(ii) Bilinearity:

$$\{aF+bG,H\} = a\{F,H\}+b\{G,H\},\quad a,b\in\mathbb{R} \tag{2.4}$$

(iii) Leibniz's Rule:

$$\{FG,H\} = \{F,H\}G + F\{G,H\} \tag{2.5}$$

(iv) Jacobi Identity:

$$\{\{F,G\},K\}+\{\{K,F\},G\}+\{\{G,K\},F\} = 0. \tag{2.6}$$

Thereby providing a realization of a Lie algebra [see, e.g., Sudarshan and Mukunda [1974] chap. 14]. A general infinite-dimensional form of this bracket, for any given two functionals $F,G\in\mathcal{B}$, can be written as follows:

$$\{\,F,G\,\} = \int_\Omega d^n z \int_\Omega d^n z'\, \mathcal{J}^{\alpha\beta}\frac{\delta F}{\delta\xi^\alpha(z)}\frac{\delta G}{\delta\xi^\beta\,(z')}\,, \tag{2.7}$$

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:

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

where α,β range over $1,2,\ldots,N$, and $\delta F/\delta\xi^\alpha$, $\delta G/\delta\xi^\beta$ are the functional derivatives defined by

$$\begin{aligned}\delta F[\xi^\alpha;\delta\xi^\alpha) &= \lim_{\epsilon\to 0}\frac{F(\xi^\alpha+\epsilon\delta\xi^\alpha)-F(\xi^\alpha)}{\epsilon}\\ &= \int_\Omega \frac{\delta F}{\delta\xi^\alpha}\delta\xi^\alpha,\end{aligned} \tag{2.8}$$

This expression can be viewed as the directional derivative of a functional F at ξ^α

in the direction $\delta\xi^\alpha$ [see, e.g., Morrison [1998b] for a formal review of these notions].

Upon inserting any functional of $\boldsymbol{\xi}$, say an observable ξ^α, into the Poisson bracket its evolution is determined by

$$\partial_t \xi^\alpha = \{\xi^\alpha, H\}\,, \tag{2.9}$$

where $H[\boldsymbol{\xi}] \in \mathcal{B}$ 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

$$\dot{H} = \{H, H\} = 0, \tag{2.10}$$

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 $\mathfrak{C}$ that satisfy

$$\{F, \mathfrak{C}\} = 0 \tag{2.11}$$

for any functional F, and thus are constants of motion for any Hamiltonian.

We will see later that to describe a dynamic in infinite-dimensional. one must select the Hamiltonian functional and a Casimir invariant to serve as entropy and construct the noncanonical Poisson bracket (2.7). First, the choice of the Hamiltonian and Casimir invariant functionals is based on the physics of the phenomena one wishes to describe. However, across all the cases we examine, the Hamiltonian functional is the total energy of the system and the usual total entropy of the system is a Casimir invariant. Second, to construct the noncanonical Poisson bracket (2.7) that consist with the choice of the Hamiltonian functional, there is a huge literature on this for a variety of systems, e.g., Morrison and Greene [1980], Morrison [1982, 1998b], Thiffeault and Morrison [2000], Abdelhamid et al. [2015], D'Avignon et al. [2016], Coquinot and Morrison [2020b], Morrison and Updike [2024], Sato and Morrison [2024] give Poisson brackets for a great many systems, including fluid dynamics, magneto-fluid dynamics, two-phase fluid dynamics, plasma kinetic theory and so one.

2.2 METRIPLECTIC FORMALISM

Metriplectic dynamics was established in the 1980s [Morrison, 1984b,a, 1986] to provide a framework for describing joined Hamiltonian and dissipative dynamics with the property that thermodynamic consistency is guaranteed. (See Kaufman and Morrison [1982], Kaufman [1984], Morrison and Hazeltine [1984], Grmela [1984b] 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 in [Öttinger and Grmela, 1997, Grmela and Öttinger, 1997] for a framework that is equivalent to metriplectic dynamics (see page 11 of Morrison and Updike [2024]). In a sequence of works [Öttinger and Grmela, 1997, Grmela and Öttinger, 1997, Öttinger, 2005] these authors were the first to explicitly incorporate ideas from non-equilibrium thermodynamics (e.g. de Groot and Mazur [1962]) into the framework. Specifically, Onsager's reciprocal relations [Onsager, 1931, Casimir, 1945] were employed to ensure entropy production. More recently, the same connection between non-equilibrium thermodynamics theory and metriplectic dynamics was made in [Coquinot and Morrison, 2020a] for a general class of magnetofluid models and more generally in [Morrison and Updike, 2024] where the metriplectic 4-bracket, a convenient quantity for constructing thermodynamically consistent systems, was introduced.

In the theory of non-equilibrium thermodynamics, it is assumed that the fluxes, say $\mathbf{J}^\alpha$, are typically linear functions of thermodynamic forces (sometimes called *affinities*), say X_β; i.e.,

$$\mathbf{J}^\alpha = L^{\alpha\beta} X_\beta \,, \tag{2.12}$$

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. We will see in the next section that one uses (2.12) to construct the so-called Metriplectic 2-bracket, which leads to describe the dissipative part of the dynamics in the infinite-dimensional.

2.2.1 METRIPLECTIC 4-BRACKET FORMALISM

The metriplectic 4-bracket theory was introduced by Morrison and Updike [2023] to describe the dissipative dynamic. Here, we 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 (2.1). We define the 4-bracket on functionals as

$$(\,\cdot\,,\,\cdot\,;\,\cdot\,,\,\cdot\,)\colon \mathcal{B}\times\mathcal{B}\times\mathcal{B}\times\mathcal{B}\to\mathcal{B} \tag{2.13}$$

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

$$(F,K;G,N)=\int_\Omega d^nz\int_\Omega d^nz'\int_\Omega d^nz''\int_\Omega d^nz'''\,\hat{R}^{\alpha\beta\gamma\delta}\times\frac{\delta F}{\delta\xi^\alpha(z)}\frac{\delta K}{\delta\xi^\beta\,(z')}\frac{\delta G}{\delta\xi^\gamma\,(z'')}\frac{\delta N}{\delta\xi^\delta\,(z''')}\,, \tag{2.14}$$

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:

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

where $\alpha,\beta,\gamma,\delta$ range over $1,2,\ldots,N$. The 4-bracket is assumed to satisfy the following proprieties:
(i) Linearity in all arguments, e.g, for all $\lambda\in\mathbb{R}$

$$(F+\lambda H,K;G,N)=(F,K;G,N)+\lambda(H,K;G,N) \tag{2.15}$$

(ii) The algebraic symmetries

$$(F,K;G,N)=-(K,F;G,N) \tag{2.16}$$
$$(F,K;G,N)=-(F,K;N,G) \tag{2.17}$$
$$(F,K;G,N)=(G,N;F,K) \tag{2.18}$$

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

$$(FH,K;G,N)=F(H,K;G,N)+(F,K;G,N)H\,. \tag{2.19}$$

Here, as usual, FH denotes point-wise multiplication. In addition, to ensure entropy production we require

$$\dot{S} = (S, H; S, H) \geq 0\,. \tag{2.20}$$

Metriplectic 4-brackets that satisfy (2.15)–(2.20) are called *minimal metriplectic*. In Sec.2.2.1 we will give a construction that ensures such appropriate positive semidefiniteness.

The minimal metriplectic properties of metriplectic 4-brackets are reminiscent of the algebraic properties possessed by a curvature tensor. In fact, every Riemannian manifold naturally has a metriplectic 4-bracket, and $(S, H; S, H)$ provides a notion of sectional curvature [see Morrison and Updike, 2023].

From the metriplectic 4-bracket (2.14), the dissipative dynamics of an observable o is generated as follows:

$$\partial_t o = (o, H; S, H) = \int d^n z \int d^n z' \int d^n z'' \int d^n z''' \, \hat{R}^{\alpha\beta\gamma\delta} \times \frac{\delta o}{\delta \xi^\alpha(z)} \frac{\delta H}{\delta \xi^\beta(z')} \frac{\delta S}{\delta \xi^\gamma(z'')} \frac{\delta H}{\delta \xi^\delta(z''')}\,. \tag{2.21}$$

If we choose o to be the Hamiltonian H, then

$$\dot{H} = (H, H; S, H) \equiv 0, \tag{2.22}$$

by the antisymmetry condition of (2.16). If we choose o to be the entropy S, then according to (2.20) we have

$$\dot{S} = (S, H; S, H) \geq 0. \tag{2.23}$$

The dissipative dynamics generated by 4-bracket on our set of field variables $\boldsymbol{\xi}$ is given by

$$\partial_t \xi^\alpha(z) = (\xi^\alpha, H; S, H) \tag{2.24}$$

$$= \int d^n z''\, G^{\alpha\beta}(z, z'') \frac{\delta S}{\delta \xi^\beta(z'')}\,, \tag{2.25}$$

where the G-metric is given as follows:

$$G^{\alpha\gamma}(z, z'') \coloneqq \int d^n z' \int d^n z''\, R^{\alpha\beta\gamma\delta}(z, z', z'', z''') \times \frac{\delta H}{\delta \xi^\beta(z')} \frac{\delta H}{\delta \xi^\delta(z''')}\,, \tag{2.26}$$

here we use the fact that $\frac{\delta \xi^\alpha(z)}{\delta \xi^\beta(z')} = \delta_{\alpha\beta}\delta(z - z')$ were $\delta_{\alpha\beta}$ is the Kronecker symbol and

$\delta(z - z^{'}))$ is the Dirac delta function. For the full metriplectic dynamics we would add the Poisson bracket (2.7) contribution to the above. Equation (2.25) is written so as to show that it amounts to a gradient system with the entropy S as generator.

$$\begin{aligned}\partial_t \xi^\alpha(z) &= \{\xi^\alpha, H\} + (\xi^\alpha, H; S, H) \\ &= \int d^n z''\, \mathcal{J}^{\alpha\beta}(z, z'') \frac{\delta H}{\delta \xi^\beta(z'')} + \int d^n z''\, G^{\alpha\beta}(z, z'') \frac{\delta S}{\delta \xi^\beta(z'')}\,, \end{aligned} \tag{2.27}$$

General Kulkarni-Nomizu construction

We can easily create specific metriplectic 4-brackets that have the minimal metriplectic properties: the requisite symmetries and the positive semidefiniteness $(S, H; S, H) \geq 0$. We do this by using the Kulkarni-Nomizu (K-N) product [Kulkarni, 1972, Nomizu, 1971]. See also Fiedler [2003] for relevant theorems. Consistent with the bracket formulation of (2.14), we deviate from the conventional K-N product by working on the dual. Given two symmetric operator fields, say Σ and M, operating on the variational derivatives; we again use the subscript notation when convenient,

$$F_\xi \coloneqq \frac{\delta F}{\delta \xi} = \left(\frac{\delta F}{\delta \xi^1}, \frac{\delta F}{\delta \xi^2}, \ldots, \frac{\delta F}{\delta \xi^N} \right)\,,$$

the K-N product is defined as follows:

$$\begin{aligned}(\Sigma \wedge M)\,(dF, dK, dG, dN) = &\,\Sigma\,(dF, dG)\, M\,(dK, dN) \\ &- \Sigma\,(dF, dN)\, M\,(dK, dG) \\ &+ M\,(dF, dG)\, \Sigma\,(dK, dN) \\ &- M\,(dF, dN)\, \Sigma\,(dK, dG)\,. \end{aligned} \tag{2.28}$$

A finite-dimensional form of Σ would be a symmetric contravariant 2-tensor, say γ, and this would give the term

$$\gamma(df, dg) = \gamma^{ij} \frac{\partial f}{\partial z^i} \frac{\partial g}{\partial z^j}\,. \tag{2.29}$$

A conventional for K-N product would involve rank 2 covariant tensors. The form of (2.29) suggests a general form in infinite dimensions would be

$$\Sigma(dF, dG) = \int d^n z \int d^n z'\, \Sigma^{\alpha\beta}(z, z') \frac{\delta F}{\delta \xi^\alpha(z)} \frac{\delta G}{\delta \xi^\beta(z')}\,, \tag{2.30}$$

where $\Sigma^{\alpha\beta}(z,z')$ is symmetric in both α,β and z,z' and operates to the right on both functional derivatives. For example,

$$\Sigma^{\alpha\beta}(z,z') = L^{\alpha\beta}_{ab}(z,z')\mathcal{L}^a\mathcal{L}'^b\,, \tag{2.31}$$

where $L^{\alpha\beta}_{ab}$ is symmetric and $\mathcal{L}^a$ is a differential operator. This implies, e.g.,

$$\Sigma(dF,dG) = \int d^nz\int d^nz'\, L^{\alpha\beta}_{ab}(z,z') \times \mathcal{L}^a\frac{\delta F}{\delta\xi^\alpha(z)}\,\mathcal{L}'^b\frac{\delta G}{\delta\xi^\beta(z')}\,. \tag{2.32}$$

With an expression for M similar to (2.30), a term in the K-N decomposition would have the following form:

$$\begin{aligned}(F,K;G,N) = \int d^nz\int d^nz'\int d^nz''\int d^nz'''\,\Sigma^{\alpha\beta}(z,z')\,M^{\gamma\delta}(z'',z''') \\ \times\ \frac{\delta F}{\delta\xi^\alpha(z)}\frac{\delta G}{\delta\xi^\beta(z')}\,\frac{\delta K}{\delta\xi^\gamma(z'')}\frac{\delta N}{\delta\xi^\delta(z''')}\ + \text{other terms}\,,\end{aligned} \tag{2.33}$$

which could be generalized further by adding filtering kernels.

Semidefinite curvature

In this section, we provide a necessary condition that ensures the non-negativity of the sectional curvature. The sectional curvature associated with two functionals F and G is defined by

$$K(F,G) = (F,G;F,G).$$

We will show that the non-negativity of this sectional curvature implies entropy production–second law of thermodynamic, i.e.,

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

We define the binary operations $\langle\cdot,\cdot\rangle_\Sigma$ and $\langle\cdot,\cdot\rangle_M$ that satisfy all of the axioms of an inner product space, except the non-degeneracy condition

$$\begin{aligned}\langle F,G\rangle_\Sigma &:= \int d^nz\int d^nz'\,\Sigma^{\alpha\beta}(z,z')\frac{\delta F}{\delta\xi^\alpha(z)}\frac{\delta G}{\delta\xi^\beta(z')}\,,\\ \langle F,G\rangle_M &:= \int d^nz''\int d^nz'''\,M^{\gamma\delta}(z'',z''')\frac{\delta F}{\delta\xi^\gamma(z'')}\frac{\delta G}{\delta\xi^\delta(z''')}\,,\end{aligned}$$

where Σ and M are positive semi-definites. We have the Cauchy-Schwarz inequality

$$|\langle F, G\rangle_\Sigma| \leq \sqrt{\langle F, F\rangle_\Sigma}\ \sqrt{\langle G, G\rangle_\Sigma} = \|F\|_\Sigma \|G\|_\Sigma \,.$$

Lemma 1. *A metriplectic quadravector constructed using the $K-N$ product, has non-negative sectional curvature,*

$$\begin{aligned} K(F,G) =& \int d^n z \int d^n z' \int d^n z'' \int d^n z''' \, \Sigma^{\alpha\beta}(z,z')\, M^{\gamma\delta}(z'',z''') \\ &\times \ \frac{\delta F}{\delta \xi^\alpha(z)} \frac{\delta F}{\delta \xi^\beta(z')} \frac{\delta G}{\delta \xi^\gamma(z'')} \frac{\delta G}{\delta \xi^\delta(z''')} \ + \ \text{other terms}\,. \end{aligned}$$

Proof. Direct calculation gives

$$K(F,G) = \|F\|_\Sigma^2 \|G\|_M^2 - 2\langle F, G\rangle_\Sigma \langle F, G\rangle_M + \|G\|_\Sigma^2 \|F\|_M^2 \,.$$

The following inequality

$$\left(\|F\|_\Sigma \|G\|_M - \|G\|_\Sigma \|F\|_M\right)^2 \geq 0$$

implies

$$\begin{aligned} \|F\|_\Sigma^2 \|G\|_M^2 + \|G\|_\Sigma^2 \|F\|_M^2 &\geq 2\|F\|_M \|F\|_\Sigma \|G\|_M \|G\|_\Sigma \\ &\geq 2\,|\langle F, G\rangle_\Sigma|\,|\langle F, G\rangle_M| \\ &\geq 2\langle F, G\rangle_\Sigma \langle F, G\rangle_M \,, \end{aligned}$$

where the second inequality follows from the Cauchy-Schwarz inequality. Evidently, the last inequality implies $K(F,G) \geq 0$ for all F and G. □

Lemma 2. *We suppose that Σ is positive definite, defining an inner product. Given any two Σ-arbitrary linearly independent $\delta F/\delta\xi$ and $\delta G/\delta\xi$, then the sectional curvature is strictly positive ($K(F,G) > 0$).*

Proof. Since $\delta F/\delta\xi$ and $\delta G/\delta\xi$ are Σ-Linearly independent, the Cauchy-Schwarz inequality given by

$$|\langle F, G\rangle_\Sigma| < \|F\|_\Sigma \|G\|_\Sigma \,.$$

In the same way we have

$$\left(\|F\|_\Sigma \|G\|_M - \|G\|_\Sigma \|F\|_M\right)^2 \geq 0$$

implies

$$\begin{aligned}\|F\|_\Sigma^2\|G\|_M^2 + \|G\|_\Sigma^2\|F\|_M^2 &\geq 2\|F\|_M\|F\|_\Sigma\|G\|_M\|G\|_\Sigma \\ &> 2\left|\langle F,G\rangle_\Sigma\right|\left|\langle F,G\rangle_M\right| \\ &> 2\langle F,G\rangle_\Sigma\langle F,G\rangle_M\,.\end{aligned}$$

Hence, we deduce that $K(F,G) > 0\,.$ □

Finite-dimensional versions of these two lemmas were first reported in [Morrison and Updike, 2023]. We notice that it is easy to see that brackets constructed with this K-N product will have all of the algebraic symmetries described in Sec.2.2.1. In addition, it is shown in previous lemmas 1 and 2 using the Cauchy-Schwarz inequality that positivity of $(S,H;S,H)$ is satisfied, if both Σ and M are positive semidefinite. Moreover, if one of Σ or M is positive definite, defining an inner product, then the sectional curvature satisfies

$$K(S,H) := (S,H;S,H) \geq 0, \tag{2.34}$$

with equality if and only if $\delta S/\delta\xi \propto \delta H/\delta\xi$. Thus, it is not difficult to build minimal metriplectic 4-brackets.

Alternative to (2.30) we can define $\Sigma(dF,dG)$ pointwise as

$$\begin{aligned}\Sigma(dF,dG)(z) &:= \int d^nz'\,\Sigma^{\alpha\beta}(z,z')\frac{\delta F}{\delta\xi^\alpha(z)}\frac{\delta G}{\delta\xi^\beta(z')} \\ &= A^{\alpha\beta}(z)\frac{\delta F}{\delta\xi^\alpha(z)}\frac{\delta G}{\delta\xi^\beta(z)}\,,\end{aligned} \tag{2.35}$$

which could follow from (2.30) if we added an additional argument to Σ. Then, with a corresponding form for M the algebraic curvature symmetries would be induced in the integrand. This is the case for our present purposes, where we assume the specific K-N form given in [Morrison and Updike, 2023], viz. where the 4-bracket is given by

$$(F,K;G,N) = \int d^nz\,W\,(\Sigma\wedge M)\,(dF,dK,dG,dN)\ ,$$

where W is an arbitrary weight, possibly depending on $\boldsymbol{\xi}$ and z, that multiplies $(\Sigma\wedge M)$ where all of the functional derivatives are evaluated at the same point, z.

The 4-bracket tool plays a crucial role in the dissipative description of dynamics, provided it satisfies certain properties that 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 (2.7) 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 (2.15)-(2.19) 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

$$K(H,S) \geq 0\,. \tag{2.36}$$

Now, for any observable functional of $\boldsymbol{\xi}$, say ξ^α, its evolution is prescribed by

$$\partial_t \xi^\alpha = \{\xi^\alpha, H\} + (\xi^\alpha, H; S, H)\,. \tag{2.37}$$

Thus we have thermodynamic consistency because:

First law (energy conservation):

$$\dot{H} = \{H,H\} + (H,H;S,H) \equiv 0\,, \tag{2.38}$$

Second law (entropy production):

$$\begin{aligned} \dot{S} &= \{S,H\} + (S,H;S,H) \\ &= 0 + K(H,S) \geq 0\,, \end{aligned} \tag{2.39}$$

where (2.38) follows from the antisymmetry condition of (2.16) and (2.39) follows from (2.36), i.e., that the sectional curvature is non-negative.

In Sec. 2.4, we will propose an unambiguous method for choosing the operators M and Σ, and thereby giving 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 one, are particular cases. We will see our construction can significantly generalize systems in the literature.

2.3 METRIPLECTIC 2-BRACKET AND CONVENTIONAL FLUXES AND AFFINITIES

For completeness we demonstrate two things in this subsection: how the metriplectic 4-bracket formalism relates to the original binary metriplectic formalism given in [Morrison, 1984b,a, 1986] and how it relates to conventional nonequilibrium thermodynamics, making the connection between the 4-bracket K-N construction and the phenomenology of thermodynamics fluxes and thermodynamic forces (or "affinities") (see equation (2.12)).

2.3.1 METRIPLECTIC 2-BRACKET

As noted above we are concerned with the metriplectic dynamics introduced in [Morrison, 1984b,a, 1986] [see also Morrison, 2009, Coquinot and Morrison, 2020b], but we mention that other binary brackets for describing dissipation were presented over the years [e.g. Kaufman and Morrison, 1982, Kaufman, 1984, Morrison and Hazeltine, 1984, Grmela, 1984a, Grmela and Öttinger, 1997, Beris and Edwards, 1994, Edwards, 1998]. In addition we mention a recent alternative approach to multiphase fluids, one based on constrained variational principles, that is given in Eldred and Gay-Balmaz [2020]. For more details, we refer the reader to Morrison and Updike [2023] for comparisons with other formulations and how they emerge from the metriplectic 4-bracket.

Metriplectic dynamics was introduced as a means of building thermodynamically consistent theories in terms of a binary bracket, which we now call the metriplectic 2-bracket. The theory applies to a wide class of dynamical systems, including both ordinary and partial differential equations. Evolution of an observable o using the metriplectic 2-bracket has the following form:

$$\partial_t o = \{o, \mathcal{F}\} - (o, \mathcal{F})_H \,, \tag{2.40}$$

where as before $\{\,.\,\}$ is the noncanonical Poisson bracket that generates the ideal part of the dynamics, while now $(F, G)_H$, the metriplectic 2-bracket, generates the dissipative part. The functional $\mathcal{F}$ represents the global Helmholtz free energy of

the system, and is given by:

$$\mathcal{F} = H - \mathcal{T}S\,, \tag{2.41}$$

where again H is the Hamiltonian and S the entropy selected from the set of Casimirs of the noncanonical Poisson bracket (ensuring $\{F, S\} = 0$ for any functional F), and $\mathcal{T}$ is a uniform nonnegative constant (a global temperature). The metriplectic 2-bracket $(\,,\,)$ is assumed to be bilinear, symmetric, and satisfies

$$(F, H)_H \equiv 0 \quad \text{for any functional } F. \tag{2.42}$$

Thus, metriplectic systems are thermodynamically consistent:

First law (energy conservation):

$$\begin{aligned} \dot{H} &= \{H, \mathcal{F}\} - (H, \mathcal{F})_H \\ &= \{H, H\} + \mathcal{T}(H, S)_H = 0\,; \end{aligned} \tag{2.43}$$

Second law (entropy production):

$$\begin{aligned} \dot{S} &= \{S, \mathcal{F}\} - (S, \mathcal{F})_H \\ &= -(S, H)_H + \mathcal{T}(S, S)_H \qquad (2.44) \\ &= \mathcal{T}(S, S)_H \geq 0\,, \qquad (2.45) \end{aligned}$$

which follows because $\{S, \mathcal{F}\} \equiv 0$ and $(S, H)_H \equiv 0$. As shown in Morrison and Updike [2023] the metriplectic 2-bracket emerges from the 4-bracket as follows:

$$(F, G)_H = (F, H; G, H)\,, \tag{2.46}$$

where for convenience here and henceforth we set $\mathcal{T} = 1$. Because of the minimal metriplectic properties of the 4-bracket, we are assured to have the thermodynamic consistency of (2.43) and (2.45).

The 2-bracket that emerges from the general 4-bracket of (2.33) is the following:

$$\begin{aligned} (F, G)_H =& (F, H; G, H) \\ =& \int d^n z \int d^n z' \int d^n z'' \int d^n z'''\, \Sigma^{\alpha\beta}(z, z')\, M^{\gamma\delta}(z'', z''') \times \frac{\delta F}{\delta \xi^\alpha(z)} \frac{\delta G}{\delta \xi^\beta(z')} \frac{\delta H}{\delta \xi^\gamma(z'')} \frac{\delta H}{\delta \xi^\delta(z''')}\,, \end{aligned} \tag{2.47}$$

which in light of the K-N product satisfies $(F,H)_H = 0$ for all F. This will be true for any choice of the Hamiltonian H. Another 2-bracket can be obtained from (2.33) by making a convenient choice of variables; viz., we choose the set of variable as in (2.1):

$$\boldsymbol{\xi}(\mathbf{z},t) = \big(\xi^1(\mathbf{z},t), \xi^2(\mathbf{z},t), \ldots, \xi^N(\mathbf{z},t)\big) \tag{2.48}$$

where the total energy density is used to be ξ^N instead of the entropy density the last dynamical variables. That this is possible is well known in thermodynamics because the entropy must be a monotonic increasing function of the internal energy, which allows via the inverse function theorem transformation between the extensive energy or extensive entropy representations [Callen, 1966]. The Hamiltonian functional is given by

$$H = \int_\Omega \xi^N \,, \tag{2.49}$$

$\delta H(z)/\delta\xi_\alpha(z') = \delta_{\alpha N}\delta(z-z')$ and $\nabla\delta H(z)/\delta\xi_\alpha(z) \equiv 0$. Thus, (2.47) reduces to

$$\begin{aligned}(F,G)_H =& (F,H;G,H)\\ =& \int d^n z \int d^n z'\, \Sigma^{\alpha\beta}(z,z') \;\times\; \frac{\delta F}{\delta\xi^\alpha(z)}\frac{\delta G}{\delta\xi^\beta(z')}\,,\end{aligned} \tag{2.50}$$

From (2.31), we set the following particular choices

$$L^{\alpha\beta}_{ab}(z,z') = L^{\alpha\beta}\delta(z-z'), \;\text{ and }\qquad \mathcal{L}^a = \mathcal{L}'^a := \nabla\,, \tag{2.51}$$

where $L^{\alpha\beta}$ are the coefficients that we will link to (2.12) in the next section. The metriplectic 2-bracket (2.50) becomes

$$(F,G)_H = (F,H;G,H) = \int_\Omega d^n z\, \nabla F_{\xi^\alpha}\cdot L^{\alpha\beta}\cdot \nabla G_{\xi^\beta}\,, \tag{2.52}$$

In Sec.2.3.2 we will give a method to build a metriplectic 2-bracket as presented in Coquinot and Morrison [2020b] and show how the bracket of (2.52) fits into the framework of conventional non-equilibrium thermodynamics as, e.g., described in de Groot and Mazur [1962]. In this way we will physically identify the meaning of $L^{\alpha\beta}$.

2.3.2 FLUXES AND AFFINITIES

In this section, we give a method introduced by Coquinot and Morrison [2020b] that lead to build the metriplectic 2-bracket. A fundamental equations of non-equilibrium thermodynamics is the general thermodynamic identity

$$\mathrm{d}\sigma = X_\alpha \mathrm{d}\xi^\alpha, \tag{2.53}$$

which relates σ, the entropy density, to the ξ^α densities associated with conserved extensive properties and to $X^\alpha \coloneqq \partial\sigma/\partial\xi^\alpha$, quantities called affinities (or thermodynamic forces). All the densities are characterized by the following conservation equations:

$$\partial_t \xi_\alpha + \nabla \cdot \mathbf{J}_\alpha = 0\,, \tag{2.54}$$

where $\mathbf{J}_\alpha$ is at present an unknown flux associated with the density ξ^α. Then, the evolution of the entropy is given by

$$\partial_t \sigma + \nabla \cdot (X_\alpha \mathbf{J}_\alpha) = \mathbf{J}_\alpha \cdot \nabla X_\alpha\,. \tag{2.55}$$

The righthand side of (2.55) is the dissipative term, which is the sum of the fluxes $\mathbf{J}_\alpha$ contracted with ∇X_α. The linear assumption of non-equilibrium processes amounts to relating fluxes and affinities according to (2.12)

$$\mathbf{J}_\alpha = L^{\alpha\beta} X_\beta\,. \tag{2.56}$$

If we identify the $L^{\alpha\beta}$ of (2.56) with that of (2.52), we see how metriplectic brackets are related to the flux-affinity relations. Onsager symmetry, assumed to arise from microscopic reversibility, amounts to the symmetry $L^{\alpha\beta} = L^{\beta\alpha}$ and the semi-definiteness property assures the second law, i.e., entropy growth.

To see how L is related to a bracket on the phase space, let us rewrite the evolution equations, at a space point $\boldsymbol{x}$ and time t, as follows:

$$\partial_t \xi^\alpha(z,t) = -\nabla \cdot \mathbf{J}_\alpha(z,t) \tag{2.57}$$

$$\begin{aligned}
&= -\nabla \cdot \left[L^{\alpha\beta}(z,t) \cdot \nabla \left(\frac{\partial \sigma}{\partial \xi^\beta} \right)(z,t) \right] \\
&= -\int_\Omega d^n z' \delta(z-z') \nabla \cdot \left[L^{\alpha\beta}(z',t) \cdot \nabla \left(\frac{\partial \sigma}{\partial \xi^\beta} \right)(z',t) \right] \\
&= \int_\Omega d^n z' \left[\nabla \left(\delta(z-z') \right) \cdot L^{\alpha\beta}(z',t) \cdot \nabla \left(\frac{\partial \sigma}{\partial \xi^\beta} \right)(z',t) \right] \\
&= \int_\Omega d^n z' \left[\nabla \left(\frac{\delta \xi^\alpha(z,t)}{\delta \xi^\gamma(z',t)} \right) \cdot L^{\gamma\beta}(z',t) \cdot \nabla \left(\frac{\delta S(t)}{\delta \xi^\beta(z',t)} \right) \right]
\end{aligned} \tag{2.58}$$

where we have used repeated index notation for summation over β and γ. Thus, the dissipation part of the dynamics can be expressed with the following symmetric 2-bracket

$$\begin{aligned}
(F,G) :&= \int_\Omega d^n z \nabla \left(\frac{\delta F}{\delta \xi^\alpha(z)} \right) \cdot L^{\alpha\beta} \cdot \nabla \left(\frac{\delta G}{\delta \xi^\beta(z)} \right) \\
&= \int_\Omega d^n z \nabla F_{\xi^\alpha} \cdot L^{\alpha\beta} \cdot \nabla G_{\xi^\beta}
\end{aligned} \tag{2.59}$$

which match with the 2-bracket (2.52) that comes from the form 4-bracket have constructed using K-N product with the choice (2.51), i.e

$$(F,G) \equiv (F,G)_H \,. \tag{2.60}$$

In the Sec.3.3.4, we will give an example of metriplectic 2-bracket formulation using the previous method.

2.4 DERIVATION OF METRIPLECTIC 4-BRACKETS

As we mentioned in Sec.2.2.1, the construction of metriplectic 4-bracket facilitated by making use of the Kulkarni-Nomizu product [Kulkarni, 1972, Nomizu, 1971] (K-N product) of two operators M and Σ. This shifts the burden to determining the two operators, which still might not be straightforward. The question of how to determine the M and Σ leads us to express the dissipative fluxes in a new manner, one different from the Onsager reciprocal relations approach of (2.12). Instead we

assume a flux-force relation as follows:

$$\mathbf{J}^{\alpha} = -L^{\alpha\beta}\,\nabla(\delta H/\delta\xi^{\beta})\,, \tag{2.61}$$

where ξ^{β} are the dynamical variables, H is the Hamiltonian functional, and $\delta H/\delta\xi^{\beta}$ is the functional derivative. We will see that expression (2.61) is intimately connected to the distinctive physical roles played by M and Σ, and it guides their determination. Expression (2.61) can be further generalized (see (2.73) below) by replacing ∇ by any pseudodifferential operator that has an adjoint, instead of a simple spatial gradient. This adjoint assumption is crucial for developing a method to derive the metriplectic 4-bracket by knowing the Hamiltonian functional H, the entropy functional S, and the unknown coefficients $L^{\alpha\beta}$. These coefficients are determined by assuming phenomenological laws, as is done with the forces in non-equilibrium thermodynamics theory [Öttinger, 2005]. This approach also has the added feature that it makes clear the origin of dependencies on dynamical and thermodynamic variables; viz., the forces that arise from $\delta H/\delta\xi^{\beta}$, which depends on internal energy functionals through H, and those that arise from phenomenological laws through $L^{\alpha\beta}$.

Systematic development of the theory

In this section we propose a method for constructing the metriplectic 4-bracket, 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. As in (2.1), the selection of set of dynamical variables defined on space-time $\Omega \times \mathbb{R}$ was defined as follows:

$$\boldsymbol{\xi}(\mathbf{z},t) = \left(\xi^{1}(\mathbf{z},t), \xi^{2}(\mathbf{z},t), \ldots, \xi^{N}(\mathbf{z},t)\right)\,, \tag{2.62}$$

where we previously commented that it is preferable to choose the ξ^{α} to be densities. To be more specific, here we suppose $\xi^{1}(\mathbf{z},t), \xi^{2}(\mathbf{z},t), \ldots, \xi^{N-1}(\mathbf{z},t)$ satisfy conservation laws and the last component ξ^{N} represent 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.3.1, Sec.3.2 and Sec.3.3 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:

$$S[\boldsymbol{\xi}] = \int_\Omega \xi^N \,. \tag{2.63}$$

This functional is required to be a Casimir invariant (see equation (2.11)) of the noncanonical Poisson bracket $\{\,\cdot,\cdot\,\}$, which one is assumed to generate the Hamiltonian part of the dynamic,

$$\{F, S\} = 0, \qquad \forall F \in \mathcal{B}\,. \tag{2.64}$$

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

$$H[\boldsymbol{\xi}] = \int_\Omega h\,, \tag{2.65}$$

where h, the Hamiltonian density, in general depends on all the variables $\xi^1, \xi^2, \ldots, \xi^N$. We will take H to be the total energy, as is indeed the case for the examples mentioned in Sec. 2.1. The evolution of the dynamical variables in the ideal case, i.e., when dissipation is not included, is given by

$$\partial_t \xi^\alpha = \{\xi^\alpha, H\}, \quad \alpha = 1, 2, \ldots, N\,. \tag{2.66}$$

Now it remains to add to (2.66) the dissipative evolution, which has the following natural combined form:

$$\partial_t \xi^\alpha = \{\xi^\alpha, H\} + \mathcal{L}^{(\alpha)} \cdot \mathbf{J}^\alpha\,, \quad \alpha = 1, \ldots, N-1\,, \tag{2.67}$$

$$\partial_t \xi^N = \{\xi^N, H\} + \mathcal{L}^{(N)} \cdot \mathbf{J}^N + \mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta\,. \tag{2.68}$$

Equation (2.67) 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 $\mathbf{J}^\alpha$. Recall, this was the purpose of the parenthesis. If ξ^α were a rank m tensor, then usually $\mathbf{J}^\alpha$ would be of rank $m+1$ with the contraction indicated by " $\cdot$ " 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 (2.67) is manifest. Equation (2.68) 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" $\mathbf{Z}_\alpha$ 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

$$\dot{S} = \int_\Omega \mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta =: \int_\Omega \dot{s}^{prod} \geq 0\,. \tag{2.69}$$

The construction above is similar to that presented in [Coquinot and Morrison, 2020a, 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 *anlysis-synthesis* method, the *analysis phase*. With this method we work backwards from the desired form of the dynamical equations (2.67) and (2.68). In the second step, the *synthesis phase*, we determine explicitly the quantities $\mathbf{J}^\alpha$, $\mathbf{Z}_\alpha$ 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 $F[\boldsymbol{\xi}]$, we have the basic identity

$$\dot{F}[\boldsymbol{\xi}] = \int_\Omega \frac{\delta F}{\delta \xi^\alpha}\, \partial_t \xi^\alpha\,, \tag{2.70}$$

which follows upon assuming Ω is fixed and boundary terms vanish, which we have assumed throughout. Applying this to H and using our notation $H_{\xi^\alpha} = \delta H/\delta \xi^\alpha$ we obtain upon substitution of (2.67) and (2.68)

$$\begin{aligned}\dot{H}[\boldsymbol{\xi}] &= \int_\Omega H_{\xi^\alpha}\, \mathcal{L}^{(\alpha)} \cdot \mathbf{J}^\alpha + H_{\xi^N}\, \mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta \\ &= \int_\Omega \mathbf{J}^\alpha \cdot \mathcal{L}^{(\alpha)}_*\, H_{\xi^\alpha} + H_{\xi^N}\, \mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta\,. \end{aligned} \tag{2.71}$$

To ensure energy conservation, (2.71) must vanish. Simple and natural choices that achieve this are the following generalized force-flux relations:

$$\mathbf{Z}_\alpha = \mathcal{L}^{(\alpha)}_* H_{\xi^\alpha}\,, \tag{2.72}$$

$$\mathbf{J}^\alpha = -H_{\xi^N} \tilde{L}^{\alpha\beta} \mathcal{L}^{(\beta)}_* H_{\xi^\beta}\,. \tag{2.73}$$

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

$$\mathbf{Z}_\alpha = \nabla H_{\xi^\alpha} \,, \tag{2.74}$$

$$\mathbf{J}^\alpha = -H_{\xi^N} \tilde{L}^{\alpha\beta} \nabla H_{\xi^\beta} = -L^{\alpha\beta} \nabla H_{\xi^\beta} \,, \tag{2.75}$$

where in the second equality of (2.75) we have made comparison with (2.61). Thus

$$L^{\alpha\beta} = H_{\xi^N} \tilde{L}^{\alpha\beta} \tag{2.76}$$

and we see that the $L^{\alpha\beta}$ of the equation (2.61) is not the same as $\tilde{L}^{\alpha\beta}$ of (2.68). 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.,

$$\tilde{L}^{\alpha\beta} = L^{\alpha\beta}/T \,. \tag{2.77}$$

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 the following choices:

$$M(dF, dG) = F_{\xi^N} \, G_{\xi^N} \,, \tag{2.78}$$

$$\begin{aligned} \Sigma(dF, dG) &= \mathcal{L}_*^{(\alpha)}(F_{\xi^\alpha}) \tilde{L}^{\alpha\beta} \mathcal{L}_*^{(\beta)}(G_{\xi^\beta}) \\ &= \mathcal{L}_*^{(\alpha)}(F_{\xi^\alpha}) \frac{L^{\alpha\beta}}{H_{\xi^N}} \mathcal{L}_*^{(\beta)}(G_{\xi^\beta}) \,. \end{aligned} \tag{2.79}$$

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

$$(F, K; G, N) = \int_\Omega (\Sigma \wedge M) \, (dF, dK, dG, dN) \,, \tag{2.80}$$

gives (2.67) and (2.68), in metriplectic form, viz.

$$\partial_t \xi^\alpha = \{ \, \xi^\alpha, H \, \} + (\xi^\alpha, H; S, H), \quad \forall \alpha = 1, \ldots, N \,. \tag{2.81}$$

Manifestly, (2.38) is satisfied and, we have for (2.39)

$$\begin{aligned}\dot{S} = (S, H; S, H) = K(H, S) = \int_\Omega \Sigma(dH, dH) \\ = \int_\Omega \mathcal{L}_*^{(\alpha)}(H_{\xi^\alpha})\, \tilde{L}^{\alpha\beta} \mathcal{L}_*^{(\beta)}(H_{\xi^\beta}) \geq 0\,. \end{aligned} \tag{2.82}$$

Comparison with (2.69) reveals $\dot{s}^{prod}$ becomes

$$\begin{aligned}\dot{s}^{prod} = \Sigma(dH, dH) = \mathcal{L}_*^{(\alpha)}\,(H_{\xi^\alpha})\, \tilde{L}^{\alpha\beta} \mathcal{L}_*^{(\beta)}(H_{\xi^\beta}) \\ = \mathcal{L}_*^{(\alpha)}\,(H_{\xi^\alpha})\, \frac{L^{\alpha\beta}}{H_{\xi^N}} \mathcal{L}_*^{(\beta)}(H_{\xi^\beta})\,. \end{aligned} \tag{2.83}$$

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 (2.78) endows Σ with the physical meaning inherent in (2.82) and (2.83) relating entropy production and sectional curvature. We comment further on these coefficients in the context of non-equilibrium thermodynamics theory in Sec. 2.4.1.

2.4.1 NON-EQUILIBRIUM THERMODYNAMICS THEORY

Many phenomena can be described by the idea that fluxes are caused by gradients of quantities, which are viewed as thermodynamic forces (affinities). 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 non-equilibrium 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 [Onsager, 1931, Casimir, 1945], which are here represented by the force-flux relations of (2.12) (see, e.g., de Groot and Mazur [1962]).

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 [Miller, 1960] and in this way the $L^{\alpha\beta}$ are provided. How-

ever 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. 2.4, we observe from equation (2.73) that the thermodynamic force-like terms now take the new form $\mathcal{L}^{(\alpha)}H_{\xi^\alpha}$, where H is the Hamiltonian functional (cf. Eq. (2.61)). In the next chapter we will confirm that our new form $\mathcal{L}^{(\alpha)}H_{\xi^\alpha}$ can match known examples and that our last set of the UT-algorithm leading to the metriplectic 4-bracket provides a mean for generalizing known examples and providing new thermodynamically consistent theories.

CHAPTER

UNIFIED THERMODYNAMIC ALGORITHM 3

In this chapter, we proposed an algorithm for constructing a metriplectic 4-bracket and, consequently, a means for producing thermodynamically consistent systems. As examples, this will be done for a general Navier-Stokes-Fourier system and for a general Cahn-Hilliard-Navier-Stokes system, a model for two phase flow. The algorithm has the following four steps: i) First, select a set of dynamical variables. ii) Next, select energy and entropy functionals, H and S, dependent on the dynamical variables, based on the physics of the phenomena to be described. iii) The third step is to obtain the noncanonical Poisson bracket [Morrison, 1998b] of the ideal (non-dissipative) part of the theory, with the chosen entropy as a Casimir invariant. iv) The final step is to construct a metriplectic 4-bracket. We will refer to the algorithm as the "unified thermodynamic algorithm" (UT-algorithm).

3.1 NAVIER-STOKES-FOURIER

As a first example we begin with the Navier-Stokes-Fourier (NSF) system. We proceed with the UT-algorithm motivated by previous development [Morrison and Updike, 2024, Zaidni et al., 2024]. En route we find the algorithm produces a significantly more general system that contains the NSF system as a special case.

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

$$\boldsymbol{\xi}(\mathbf{x},t) = (\rho(\mathbf{x},t), \mathbf{m}(\mathbf{x},t), \sigma(\mathbf{x},t))\,, \tag{3.1}$$

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 (2.62).

• Second step of UT-algorithm: Consistent with (2.63), we take the total entropy to be the integral of the last component

$$S = \int_\Omega \sigma\,. \tag{3.2}$$

For the Hamiltonian functional for NSF a natural choice would be

$$H = \int_\Omega \frac{|\mathbf{m}|^2}{2\rho} + \rho\, u(\rho, \sigma/\rho)\,, \tag{3.3}$$

the sum of fluid kinetic energy and 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 thermodynamics relations are

$$p = \rho^2 \frac{\partial u}{\partial \rho} \qquad \text{and} \qquad T = \frac{\partial u}{\partial s}\,, \tag{3.4}$$

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 that given in [Morrison and Greene, 1980]. For two functionals $F, G \in \mathcal{B}$ it is defined as follows:

$$\begin{aligned}\{F, G\} = -\int_\Omega \mathbf{m} \cdot [F_\mathbf{m} \cdot \nabla G_\mathbf{m} - G_\mathbf{m} \cdot \nabla F_\mathbf{m}] \\ + \rho\,[F_\mathbf{m} \cdot \nabla G_\rho - G_\mathbf{m} \cdot \nabla F_\rho] \\ + \sigma\,[F_\mathbf{m} \cdot \nabla G_\sigma - G_\mathbf{m} \cdot \nabla F_\sigma]\,,\end{aligned} \tag{3.5}$$

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 the systematic development theory presented in Sec. 2.4, viz., M and Σ are given

by

$$M(dF, dG) = F_\sigma \, G_\sigma \,, \tag{3.6}$$

$$\Sigma(dF, dG) = \mathcal{L}_*^{(\alpha)}(F_{\xi^\alpha}) \frac{L^{\alpha\beta}}{H_\sigma} \mathcal{L}_*^{(\beta)}(G_{\xi^\beta}) \,, \tag{3.7}$$

and the UTA is complete up to the choices for $\mathcal{L}_*^{(\alpha)}$ and $L^{\alpha\beta}$. For any choices of these quantities, according to (2.73) and (2.76), the 4-bracket using (3.6) and (3.7) will be consistent with the following general expressions for the fluxes:

$$\begin{aligned}
\mathbf{J}_\rho &= -L^{\rho\rho} \cdot \mathcal{L}_*^\rho(H_\rho) - L^{\rho\mathbf{m}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\rho\sigma} \cdot \mathcal{L}_*^\sigma(H_\sigma) \,, \\
\bar{J}_{\mathbf{m}} &= -L^{\mathbf{m}\rho} \otimes \mathcal{L}_*^\rho(H_\rho) - L^{\mathbf{mm}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\mathbf{m}\sigma} \otimes \mathcal{L}_*^\sigma(H_\sigma) \,, \\
\mathbf{J}_s &= -L^{\sigma\rho} \cdot \mathcal{L}_*^\rho(H_\rho) - L^{\sigma\mathbf{m}} : \mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\sigma\sigma} \cdot \mathcal{L}_*^\sigma(H_\sigma) \,,
\end{aligned} \tag{3.8}$$

where $\mathbf{J}_\rho$ is the net mass flux, $\bar{J}_{\mathbf{m}}$ is the momentum flux, and $\mathbf{J}_s$ is the net entropy flux. Thus we have obtained a quite general thermodynamically consistent system, one that generalizes the NSF system. In fact, the 4-bracket that produces (3.8) is sufficiently general to produce the Brenner-Navier-Stokes system of Sec. 3.2 and the significant generalizations of the BNS that we describe there.

Now we specialize and show that the general expressions for the fluxes of (3.8) reduce to those known for the NSF (see, e.g., de Groot and Mazur [1962], Coquinot and Morrison [2020b], Morrison [1984a]), viz.

$$\mathbf{J}_\rho = 0 \,, \quad \bar{J}_{\mathbf{m}} = -\bar{\bar{\Lambda}} : \nabla \mathbf{v} \,, \quad \mathbf{J}_s = -\frac{\bar{\kappa}}{T} \cdot \nabla T \,, \tag{3.9}$$

where $\mathbf{J}_\rho$ is the net (vector) mass flux, $\bar{J}_{\mathbf{m}}$ is the momentum flux (rank 2 tensor), and $\mathbf{J}_s$ is the net (vector) entropy flux. In (3.9) $\bar{\kappa}$ 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 $\bar{\bar{\Lambda}}$ is the viscosity 4-tensor, the usual rank 4 isotropic Cartesian tensor given by

$$\Lambda_{ijkl} = \eta \left(\delta_{il}\delta_{jk} + \delta_{jl}\delta_{ik} - \frac{2}{3}\delta_{ij}\delta_{kl} \right) + \zeta \, \delta_{ij}\delta_{kl} \,, \tag{3.10}$$

with viscosity coefficients η and ζ and i, j, k and l taking on values 1,2,3. In (3.9) and henceforth we use a single " $\cdot$ " to indicate neighboring contractions and we use

the double dot convention as follows:

$$\begin{aligned}(\bar{\kappa}\cdot\nabla G_\sigma)_i &= \kappa_{ij}\partial_j G_\sigma\\ (\bar{\bar{\Lambda}}:\nabla\mathbf{m})_{ij} &= \Lambda_{ijkl}\partial_k m_l\\ (\boldsymbol{\epsilon}:\nabla\mathbf{m})_i &= \epsilon_{ijk}\partial_j m_k\end{aligned} \tag{3.11}$$

where repeated indices are summed over. We have added (3.11) for later use, when we have a double contraction with a 3-tensor $\boldsymbol{\epsilon}$.

To see how the fluxes of (3.9) emerge from our general expressions of (3.8) we set $\mathcal{L}_*^{(\alpha)} = \nabla$, for all α, and assume H is given by (3.3); therefore

$$H_\sigma = T, \quad H_{\mathbf{m}} = \mathbf{v}, \quad H_\rho = -\frac{|\mathbf{m}|^2}{2\rho^2} + u - \frac{T\,\sigma}{\rho} + \frac{p}{\rho}, \tag{3.12}$$

and comparison of (3.8) with (3.9) reveals that the only nonzero phenomenological coefficients $L^{\alpha\beta}$ are the following:

$$L^{\mathbf{mm}} = \bar{\bar{\Lambda}} \quad \text{and} \quad L^{\sigma\sigma} = \frac{\bar{\kappa}}{T}\,. \tag{3.13}$$

Thus we immediately obtain Σ from (3.7) as

$$\begin{aligned}\Sigma(dF, dG) &= \nabla F_{\mathbf{m}} : \frac{L^{\mathbf{mm}}}{H_\sigma} : \nabla G_{\mathbf{m}} + \nabla F_\sigma \cdot \frac{L^{\sigma\sigma}}{H_\sigma}\cdot\nabla G_\sigma\\ &= \nabla F_{\mathbf{m}} : \frac{\bar{\bar{\Lambda}}}{T} : \nabla G_{\mathbf{m}} + \nabla F_\sigma \cdot \frac{\bar{\kappa}}{T^2}\cdot\nabla G_\sigma\end{aligned} \tag{3.14}$$

which together with the expression for M of (3.6) gives the 4-bracket

$$\begin{aligned}(F, K; G, N) = \int_\Omega \frac{1}{T}\Big[\,&[K_\sigma\nabla F_{\mathbf{m}} - F_\sigma\nabla K_{\mathbf{m}}]:\bar{\bar{\Lambda}}:[N_\sigma\nabla G_{\mathbf{m}} - G_\sigma\nabla N_{\mathbf{m}}]\\ &+\ \frac{1}{T}\left[K_\sigma\nabla F_\sigma - F_\sigma\nabla K_\sigma\right]\cdot\bar{\kappa}\cdot\left[N_\sigma\nabla G_\sigma - G_\sigma\nabla N_\sigma\right]\Big]\,.\end{aligned} \tag{3.15}$$

Insertion of H of (3.3) and S of (3.2), yields the NSF dynamical system

$$\begin{aligned}
\partial_t \rho &= \{\rho, H\} + (\rho, H; S, H) \\
&= -\mathbf{v}\cdot\nabla\rho - \rho\,\nabla\cdot\mathbf{v}\,, \qquad (3.16)\\
\partial_t \mathbf{v} &= \{\mathbf{v}, H\} + (\mathbf{v}, H; S, H) \\
&= -\mathbf{v}\cdot\nabla\mathbf{v} - \nabla p/\rho + \frac{1}{\rho}\nabla\cdot(\bar{\bar{\Lambda}} : \nabla\mathbf{v})\,, \qquad (3.17)\\
\partial_t \sigma &= \{\sigma, H\} + (\sigma, H; S, H) \\
&= -\mathbf{v}\cdot\nabla\sigma - \sigma\,\nabla\cdot\mathbf{v} + \nabla\cdot\Big(\frac{\bar{\kappa}}{T}\cdot\nabla T\Big) + \frac{1}{T^2}\nabla T\cdot\bar{\kappa}\cdot\nabla T + \frac{1}{T}\nabla\mathbf{v} : \bar{\bar{\Lambda}} : \nabla\mathbf{v}\,. \qquad (3.18)
\end{aligned}$$

Here we have dropped surface terms arising from integration by parts and have used $\delta\rho(\mathbf{x})/\delta\rho(\mathbf{x}') = \delta\sigma(\mathbf{x})/\delta\sigma(\mathbf{x}') = \delta\mathbf{v}(\mathbf{x})/\delta\mathbf{v}(\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}')$. By construction we automatically have the entropy production

$$\dot{S} = (S, H; S, H) = \int_\Omega \dot{s}^{prod} \geq 0\,. \qquad (3.19)$$

where

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

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

3.2 BRENNER-NAVIER-STOKES-FOURIER

In a series of papers [Brenner, 2005b,a, 2006, 2012] 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. 3.1. Moreover, our theory shows the following: how to unambiguously delineate the dissipative dynamics from the nondisipative (Hamiltonian) dynamics; that generalizations of Brenner's theory by other authors are again special cases of our theory, in particular they all emerge from (3.8); 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" that 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:

$$\partial\rho + \nabla\cdot(\rho\mathbf{v}_m) = 0\,, \tag{3.20}$$

$$\partial(\rho\,\mathbf{v}) + \nabla\cdot(\rho\,\mathbf{v}_m\mathbf{v}) = \nabla\cdot(-p\bar{I} + \bar{\bar{\Lambda}} : \nabla\mathbf{v})\,, \tag{3.21}$$

$$\partial\sigma + \nabla\cdot(\sigma\mathbf{v}_m) = \nabla\cdot\left[\frac{\bar{\kappa}}{T}\cdot\nabla T - \frac{\mathbf{w}}{T}\,(p + u - \rho\alpha)\right] + \dot{s}^{prod}\,.$$

Here, as before, $u(\rho, s)$ is the internal energy per unit volume, 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 [Brenner, 2005b] Brenner first proposed $\mathbf{w} = \alpha\nabla\ln(\rho)$. Later in [Brenner, 2006] and [Öttinger, 2005, Bedeaux et al., 2006], using using Öttinger's version of GENERIC, it was settled on following form for $\mathbf{w}$:

$$\mathbf{w} = \tilde{D}\,(\nabla p - \gamma\nabla T)\ ,\ . \tag{3.22}$$

where for simplicity we introduced the diffusion-like coefficient $\tilde{D} \coloneqq D'/(\rho^2 T)$ and the parameter γ is defined by

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

Thus the system contain one parameter, either α or γ. By taking $\gamma = \left(\frac{\partial p}{\partial T}\right)_\rho$, Brenner established that the difference velocity $\mathbf{w}$ becomes

$$\mathbf{w} = \frac{\tilde{D}}{\kappa_T}\nabla\ln\rho\,, \tag{3.23}$$

where $\kappa_T = \frac{1}{\rho}\left(\frac{\partial\rho}{\partial p}\right)_T$ is the coefficient of isothermal compressibility, assumed to be nonnegative. 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 [Reddy et al., 2019], 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 term of variables $\boldsymbol{\xi} = (\rho, \mathbf{m} = \rho\mathbf{v}, \sigma)$ as follows:

$$\partial_t\rho + \nabla\cdot(\rho\mathbf{v}) = \nabla\cdot(\rho\mathbf{w})\,, \tag{3.24}$$

$$\partial_t\mathbf{m} + \nabla\cdot(\mathbf{m}\otimes\mathbf{v}) = \nabla\cdot(-p\bar{I} + \bar{\bar{\Lambda}}:\nabla\mathbf{v} + \mathbf{m}\otimes\mathbf{w})\,, \tag{3.25}$$

$$\partial_t\sigma + \nabla\cdot(\sigma\mathbf{v}) = \nabla\cdot\Big[\frac{\bar{\kappa}}{T}\nabla T + (\sigma-\gamma)\mathbf{w}\Big] + \dot{s}^{prod}\,. \tag{3.26}$$

Except for γ and $\mathbf{w}$ the quantities above are defined as for the NSF system. Evidently, from (3.24), (3.25), and (3.26) it is seen that the fluxes are given by the following:

$$\mathbf{J}_\rho = -\rho\mathbf{w}\,, \tag{3.27}$$

$$\bar{J}_\mathbf{m} = -\bar{\bar{\Lambda}}:\nabla\mathbf{v} - \mathbf{m}\otimes\mathbf{w}\,, \tag{3.28}$$

$$\mathbf{J}_s = -\frac{\bar{\kappa}}{T}\cdot\nabla T - (\sigma-\gamma)\mathbf{w}\,, \tag{3.29}$$

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

Given the above and the results of Sec. 3.1, there is no need to run through the steps of the UT-algorithm: the variables $\boldsymbol{\xi}$ are the same, the forms of S and H of (3.2) and (3.3) are the same, the Poisson bracket is again the Morrison-Greene Poisson bracket of (3.5) and, the form of the operators $\mathcal{L}^{(\alpha)}$ are the same. Thus, it only remains to determine the phenomenological coefficients and these are provided by matching (3.27), (3.28) and (3.29) with (3.8).

Comparison of (3.27) with the first equation of (3.8) leads to the determination of $\mathbf{w}$. We have

$$\mathbf{J}_\rho = -L^{\rho\rho}\cdot\nabla H_\rho - L^{\rho\mathbf{m}}:\nabla H_\mathbf{m} - L^{\rho\sigma}\cdot\nabla H_\sigma\,, \tag{3.30}$$

where the 2-tensors $L^{\rho\rho}$ and $L^{\rho\sigma}$ and the 3-tensor $L^{\rho\mathbf{m}}$ are contracted as in (3.11). From the functional derivative H_ρ of (3.12) and the local thermodynamic identities (3.4) we find

$$\nabla H_\rho = -\frac{\sigma}{\rho}\nabla T + \frac{1}{\rho}\nabla p - (\nabla\mathbf{v})\cdot\mathbf{v} \tag{3.31}$$

and

$$\nabla p = \rho \nabla H_\rho + (\nabla H_{\mathbf{m}}) \cdot \mathbf{m} + \sigma \nabla H_\sigma \,. \tag{3.32}$$

Thus the difference velocity $\mathbf{w}$ of (3.22) can be rearranged as the following linear combination of ∇H_ρ, $\nabla H_{\mathbf{m}}$ and ∇H_σ:

$$\mathbf{w} = \tilde{D}\rho \, \nabla H_\rho + \tilde{D} \, (\nabla H_{\mathbf{m}}) \cdot \mathbf{m} + \tilde{D}\hat{\sigma} \, \nabla H_\sigma \,. \tag{3.33}$$

where we defined $\hat{\sigma} \coloneqq \sigma - \gamma$. Therefore, according to (3.27)

$$\mathbf{J}_\rho = -\tilde{D}\rho^2 \, \nabla H_\rho - \tilde{D}\rho \, (\nabla H_{\mathbf{m}}) \cdot \mathbf{m} - \tilde{D}\rho\hat{\sigma} \, \nabla H_\sigma \,, \tag{3.34}$$

and comparison with (3.30) yields

$$L^{\rho\rho} = \tilde{D}\rho^2 \, \bar{I} \,, \quad L^{\rho\mathbf{m}} = \tilde{D}\rho \, \bar{I} \otimes \mathbf{m} \,, \quad L^{\rho\sigma} = \tilde{D}\rho\hat{\sigma} \, \bar{I} \,. \tag{3.35}$$

Similarly, using (3.8), (3.28), and (3.33),

$$\begin{aligned} \bar{J}_{\mathbf{m}} &= -L^{\mathbf{m}\rho} \otimes \nabla H_\rho - L^{\mathbf{mm}} \colon \nabla H_{\mathbf{m}} - L^{\mathbf{m}\sigma} \otimes \nabla H_\sigma \\ &= -\bar{\bar{\Lambda}} \colon \nabla H_{\mathbf{m}} - \mathbf{m} \otimes \big(\tilde{D}\rho \, \nabla H_\rho + \tilde{D} \, (\nabla H_{\mathbf{m}}) \cdot \mathbf{m} + \tilde{D}\hat{\sigma} \, \nabla H_\sigma \big) \,; \end{aligned} \tag{3.36}$$

whence we see

$$\begin{aligned} L^{\mathbf{m}\rho} &= \tilde{D}\rho \, \mathbf{m} \,, \quad L^{\mathbf{m}\sigma} = \tilde{D}\hat{\sigma} \, \mathbf{m} \,, \quad \text{and} \\ L^{\mathbf{mm}} &= \bar{\bar{\Lambda}} + \tilde{D} \, \mathbf{m} \otimes \bar{I} \otimes \mathbf{m} \,. \end{aligned} \tag{3.37}$$

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

$$\begin{aligned} \big(\mathbf{m} \otimes \bar{I} \otimes \mathbf{m} \big) : \nabla H_{\mathbf{m}} \big)_{ij} &= (m_i \delta_{jk} m_l) \partial_k v_l \\ &= m_i m_l \partial_j v_l \,. \end{aligned} \tag{3.38}$$

Finally, using (3.8), (3.29), and (3.33),

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

whence we see

$$L^{\sigma\rho} = \tilde{D}\rho\hat{\sigma}\,\bar{I}\,, \quad L^{\sigma\sigma} = \frac{\bar{\kappa}}{T} + \tilde{D}\hat{\sigma}^2\,\bar{I} \tag{3.39}$$

$$L^{\sigma\mathbf{m}} = \tilde{D}\hat{\sigma}\,\bar{I}\otimes\mathbf{m} \tag{3.40}$$

Given phenomenological coefficients we obtain directly the operators M and Σ. Again M is chosen as in (3.6), while Σ is given as follows:

$$\begin{aligned}\Sigma(dF,dG) = \frac{1}{T}\Big[&\tilde{D}\rho^2\,\nabla F_\rho\cdot\nabla G_\rho + \tilde{D}\rho\left(\nabla F_\rho\cdot(\nabla G_{\mathbf{m}})\cdot\mathbf{m} + \nabla G_\rho\cdot(\nabla F_{\mathbf{m}})\cdot\mathbf{m}\right)\\ &+ \tilde{D}\rho\hat{\sigma}\left(\nabla F_\rho\cdot\nabla G_\sigma + \nabla G_\rho\cdot\nabla F_\sigma\right)\\ &+ \nabla F_{\mathbf{m}} : \left(\bar{\bar{\Lambda}} + \tilde{D}\,\mathbf{m}\otimes\bar{I}\otimes\mathbf{m}\right) : \nabla G_{\mathbf{m}}\\ &+ \tilde{D}\hat{\sigma}\left(\nabla F_\sigma\cdot(\nabla G_{\mathbf{m}})\cdot\mathbf{m} + \nabla G_\sigma\cdot(\nabla F_{\mathbf{m}})\cdot\mathbf{m}\right)\\ &+ \nabla F_\sigma\cdot\left(\frac{\bar{\kappa}}{T} + \tilde{D}\hat{\sigma}^2\bar{I}\right)\cdot\nabla G_\sigma\Big]\,.\end{aligned} \tag{3.41}$$

Note in the penultimate line of (3.41) we have used

$$\nabla F_\sigma\cdot\bar{I}\otimes\mathbf{m} : \nabla G_{\mathbf{m}} = \nabla F_\sigma\cdot(\nabla G_{\mathbf{m}})\cdot\mathbf{m}\,. \tag{3.42}$$

(Recall (3.11).) By the metriplectic 4-bracket $(\,.\,,\,.\,;\,.\,,\,.\,)$ that comes from the K-N product of M and Σ and upon insertion of S as given by (3.2) and H as given by (3.3), the system (3.24), (3.25), and (3.26) 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:

$$\begin{aligned}\dot{S} = (S, H;, S, H) &= \int_\Omega \Sigma(dH, dH)\\ &= \int_\Omega \frac{1}{\tilde{D}\,T}\mathbf{w}\cdot\mathbf{w} + \nabla T\cdot\frac{\bar{\kappa}}{T}\cdot\nabla T + \nabla\mathbf{v} : \bar{\bar{\Lambda}} : \nabla\mathbf{v}\\ &= \int_\Omega \frac{1}{T}\left[\tilde{D}|\mathbf{v}_m - \mathbf{v}|^2 + \nabla T\cdot\frac{\bar{\kappa}}{T}\cdot\nabla T + \nabla\mathbf{v} : \bar{\bar{\Lambda}} : \nabla\mathbf{v}\right] \geq 0\,.\end{aligned} \tag{3.43}$$

Alternatively, using (3.23)

$$\dot{S} = \int_\Omega \frac{1}{T}\left[\frac{\tilde{D}}{\kappa_T^2\rho^2}|\nabla\rho|^2 + \nabla T\cdot\frac{\bar{\kappa}}{T}\cdot\nabla T + \nabla\mathbf{v}:\bar{\bar{\Lambda}}:\nabla\mathbf{v}\right] \geq 0\,. \tag{3.44}$$

Therefore, we shown that the system proposed by Brenner [2006] 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 Morrison and Greene [1980]. 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., $\rho = const$).

We have also shown that the expression of $\mathbf{w}$ given by (3.22) is not the most general form giving a thermodynamically consistent system, since from (3.30)

$$\mathbf{w} = \big(L^{\rho\rho}\cdot\nabla H_\rho + L^{\rho\mathbf{m}}:\nabla H_\mathbf{m} + L^{\rho\sigma}\cdot\nabla H_\sigma\big)/\rho\,, \tag{3.45}$$

we see that $\mathbf{w}$ can be any linear combinations 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 $L^{\rho\mathbf{m}}$.

In a more recent paper [Reddy et al., 2019] 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. 3.1 with (3.45). Specifically, the cases of Reddy et al. [2019] (rewritten in our notation) are as follows:

Equation (77) of Reddy et al. [2019],

$$\mathbf{w} = \kappa_m\nabla\ln\rho\,, \tag{3.46}$$

where $\kappa_m = \tilde{D}/\kappa_T$, is Brenner's (3.23) using $\gamma = \left(\frac{\partial p}{\partial T}\right)_\rho$;
Equation (78) of Reddy et al. [2019],

$$\mathbf{w} = \kappa_T\nabla\ln T = \frac{\kappa_T}{T}\nabla H_\sigma\,, \tag{3.47}$$

is given by our (3.45) with the choices

$$L^{\rho\rho} = L^{\rho\mathbf{m}} = 0, \quad L^{\rho\sigma} = \rho\,\frac{\kappa_T}{T}\,\bar{I}\,; \tag{3.48}$$

Equation (79) of Reddy et al. [2019]

$$\begin{aligned}\mathbf{w} &= \kappa_p \nabla \ln p = \frac{\kappa_p}{p} \nabla p \\ &= \frac{\kappa_p}{p} \big(\rho \nabla H_\rho + (\nabla H_{\mathbf{m}}) \cdot \mathbf{m} + \sigma \nabla H_\sigma \big) \,, \end{aligned} \tag{3.49}$$

where κ_p is the thermal conductivity at constant pressure and the third equality follows from (3.32). Equation (3.49) is given by our (3.45) with the choices

$$\begin{aligned} &L^{\rho\rho} = \rho^2 \frac{\kappa_p}{p} \, \bar{I} \,, \quad L^{\rho \mathbf{m}} = \rho \, \kappa_p \, \bar{I} \otimes \mathbf{m} \,; \\ &L^{\rho\sigma} = \rho \, \kappa_p \, \sigma \, \bar{I}; \end{aligned} \tag{3.50}$$

Equation (80) of Reddy et al. [2019],

$$\mathbf{w} = \kappa_\tau \nabla \times \mathbf{v} = \kappa_\tau \nabla \times H_{\mathbf{m}} \,, \tag{3.51}$$

where κ_τ is another phenomenological quantity. Equation (3.51) is a particular case of our theory by taking

$$L^{\rho\rho} = 0, \quad L^{\rho \mathbf{m}} = \rho \, \kappa_\tau \, \boldsymbol{\epsilon} \,, \quad L^{\rho\sigma} = 0 \,. \tag{3.52}$$

where $\boldsymbol{\epsilon}$ is the Levi-Civita 3-tensor (density) and contraction is defined by (3.11). Note, the tensorial inconsistency of (3.51) can be resolved by assuming κ_T is a pseudoscalar.

3.3 GIBBS-NAVIER-STOKES

In this section we describe general features of the metriplectic framework in the context of the Gibbs-Navier-Stokes system (GNS), a generalization of the Navier-Stokes equations that includes the dual thermodynamical variables of concentration and chemical potential.

3.3.1 DESCRIPTION OF THE GIBBS-NAVIER-STOKES SYSTEM

The GNS for 2 phase flow proceeds on familiar ground [Eckart, 1940a,b, de Groot and Mazur, 1962]. It amounts to the single phase thermodynamic Navier-Stokes system or as it is sometimes called the Fourier Navier-Stokes system with the dispersed phase described by the addition of a concentration variable, c, giving the set of dynamical variables $\{\mathbf{v}, \rho, c, s\}$. Here we review global aspects of this known system, before showing how it emerges from the metriplectic formalism.

We suppose the mixture of two phases are contained in a volume Ω, and we consider the following global quantities and their evolution:

$$M = \int_\Omega \rho\,, \quad \dot{M} = -\int_{\partial\Omega} \mathbf{J}_\rho \cdot \mathbf{n}, \tag{3.53}$$

$$\mathbf{P} = \int_\Omega \rho\,\mathbf{v}\,, \quad \dot{\mathbf{P}} = -\int_{\partial\Omega} \bar{J}_{\mathbf{m}} \cdot \mathbf{n}, \tag{3.54}$$

$$H = \int_\Omega \frac{\rho}{2}\,|\mathbf{v}|^2 + \rho\,u(\rho, s, c)\,, \quad \dot{H} = -\int_{\partial\Omega} \mathbf{J}_e \cdot \mathbf{n}\,, \tag{3.55}$$

$$C = \int_\Omega \rho\,c\,, \quad \dot{C} = -\int_{\partial\Omega} \mathbf{J}_c \cdot \mathbf{n}, \tag{3.56}$$

$$S = \int_\Omega \rho\,s\,, \quad \dot{S} = -\int_{\partial\Omega} \mathbf{J}_s \cdot \mathbf{n} + \int_\Omega \dot{s}^{prod}\,. \tag{3.57}$$

Here ρ is the density of the mixture, $\mathbf{v}$ is the mass-averaged velocity of the mixture, s is the specific entropy, and the phase variable c is the specific concentration (dimensionless mass concentration) that determines how much of the dispersed phase of the mixture is present at a point $\mathbf{x} \in \Omega \subset \mathbb{R}^3$. The variable $\tilde{c} = \rho c$ is the mass density of the dispersed phase. The functionals M, P, H and S are the total mass, momentum, energy, and entropy of the mixture, respectively, while C is the total mass of one of the constituents. The local thermodynamics of the mixture is described by $u(\rho, s, c)$, the internal energy per unit mass. For convenience the gravitational force is not considered, although its inclusion is straightforward.

Quantities in the time derivatives of the basic functionals are as follows: $\mathbf{n}$ is the unit outward normal vector of the boundary $\partial\Omega$, $\mathbf{J}_\rho$ is the net mass flux, $\mathbf{J}_c$ is the phase field flux, which depends on gradient of the chemical potential, $\bar{J}_{\mathbf{m}}$ is the stress tensor – surface forces – due to pressure and viscosity, $\mathbf{J}_e$ the energy flux that contains the rate of work done by the surface forces (external energy), the rate of

heat transfer and the rate of diffusivity in phase field (internal energy), $\mathbf{J}_s$ is the net entropy flux through the boundary, and $\dot{s}^{prod}$ is the local rate of entropy production. The second law of thermodynamics is expressed by the requirement that $\dot{s}^{prod}$ is non-negative.

For the GNS system the fluxes are given by

$$\mathbf{J}_\rho = 0\,, \tag{3.58}$$

$$\mathbf{J}_c = -\bar{D}\cdot\nabla\mu\,, \tag{3.59}$$

$$\bar{J}_{\mathbf{m}} = p\,\bar{I} - \bar{\bar{\Lambda}} : \nabla\mathbf{v}\,, \tag{3.60}$$

$$\mathbf{J}_e = -\mathbf{v}\cdot\bar{\bar{\Lambda}} : \nabla\mathbf{v} - \bar{\kappa}\cdot\nabla T - \mu\bar{D}\cdot\nabla\mu\,, \tag{3.61}$$

$$\mathbf{J}_s = -\frac{\bar{\kappa}}{T}\cdot\nabla T\,, \tag{3.62}$$

$$\dot{s}^{prod} = \frac{1}{T}\Big[\nabla\mathbf{v} : \bar{\bar{\Lambda}} : \nabla\mathbf{v} + \frac{1}{T}\,\nabla T\cdot\bar{\kappa}\cdot\nabla T + \nabla\mu\cdot\bar{D}\cdot\nabla\mu\Big] \geq 0\,, \tag{3.63}$$

where p is the pressure, T is the temperature, $\bar{I}$ is the unit tensor, $\bar{\kappa}$ 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 μ is the chemical potential. We allow the possibility that phenomenological quantities such as $\bar{\kappa}$ and $\bar{D}$ can depend on the dynamical variables. Here, $\bar{\bar{\Lambda}}$ is the viscosity 4-tenor as given in (3.10).

The volume density variables are $\boldsymbol{\xi} = (\mathbf{m} \coloneqq \rho\mathbf{v}, \rho, \sigma \coloneqq \rho s, \tilde{c} \coloneqq \rho c)$, where $\mathbf{m}$ is the momentum density, σ is entropy per unit volume and $\tilde{c}$ is the concentration per unit volume. The local energy per unit volume is given by

$$e = \frac{|\mathbf{m}|^2}{2\rho} + \rho u(\rho, s, c)\,. \tag{3.64}$$

From the specific internal energy, $u(\rho, s, c)$, we have the thermodynamic relations

$$\mathrm{d}u = T\mathrm{d}s + \frac{p}{\rho^2}\mathrm{d}\rho + \mu\mathrm{d}c\,, \tag{3.65}$$

where

$$T = \frac{\partial u}{\partial s}\,, \qquad p = \rho^2\frac{\partial u}{\partial \rho}\,, \qquad \mu = \frac{\partial u}{\partial c}\,. \tag{3.66}$$

Given the content of this section, we have established the first step of UT-algorithm for the GNS system, the determination of the dynamical variables $\{\mathbf{m} = \rho\mathbf{v}, \rho, \tilde{c} = \rho c, \sigma = \rho s\}$ or alternatively the set $(\mathbf{v}, \rho, c, s)$, and the second step of UT-algorithm by making the choices of Hamiltonian H of (3.55) and entropy S of (3.57). In the next section, Sec.(3.3.2), we proceed to the third step of UT-

algorithm by obtaining the Hamiltonian structure for this system. This system without dissipation is the GE system.

3.3.2 NONCANONICAL POISSON BRACKET OF THE GIBBS-EULER SYSTEM

Given that the mixture is assumed to be confined in the domain Ω, the Eulerian scalars (volume forms) $(\rho, \tilde{c}, \sigma)$ are functions from space-time $\Omega \mapsto \mathbb{R} \to \mathbb{R}$, while the vector field $\mathbf{m}$ maps $\Omega \times \mathbb{R} \mapsto T\Omega$, where $T\Omega$ stands for the tangent bundle of the manifold Ω. We will forgo formal geometric considerations and suppose our infinite-dimensional phase space has coordinates

$$\boldsymbol{\xi} = (\mathbf{m}, \rho, \tilde{c}, \sigma)\,, \tag{3.67}$$

and observables are functionals that map $\boldsymbol{\xi} \mapsto \mathbb{R}$ at each fixed time. The appropriate Poisson bracket, defined on two functionals $F, G \in \mathcal{B}$, for the GE system is the following:

$$\begin{aligned}\{F, G\} = -\int_\Omega \mathbf{m} \cdot [F_\mathbf{m} \cdot \nabla G_\mathbf{m} - G_\mathbf{m} \cdot \nabla F_\mathbf{m}] \\ + \rho\,[F_\mathbf{m} \cdot \nabla G_\rho - G_\mathbf{m} \cdot \nabla F_\rho] \\ + \sigma\,[F_\mathbf{m} \cdot \nabla G_\sigma - G_\mathbf{m} \cdot \nabla F_\sigma] \\ + \tilde{c}\,[F_\mathbf{m} \cdot \nabla G_{\tilde{c}} - G_\mathbf{m} \cdot \nabla F_{\tilde{c}}]\,,\end{aligned} \tag{3.68}$$

where we compactified our notation by defining $F_\mathbf{m} := \delta F/\delta \mathbf{m}$, $F_\rho := \delta F/\delta \rho$, etc., the functional derivatives with respect to the various coordinates $\boldsymbol{\xi}$. That this is the appropriate Poisson bracket is immediate; it is the Lie-Poisson bracket originally given by Morrison and Greene [1980] with the addition of the last line of (3.68) involving the concentration, another volume density variable $\tilde{c}$. Adding such a dynamical variable is common place in the fluid modeling of plasmas over the last decades and fits within the general theory for extension given by Thiffeault and Morrison [2000]. By construction we have a Poisson bracket that is a bilinear, antisymmetric, and either by the extension theory or a relatively easy direct calculation using the techniques of Morrison [1982] it can be shown to satisfy the Jacobi identity, i.e.,

$$\{\{F, G\}, H\} + \{\{H, F\}, G\} + \{\{G, H\}, F\} = 0\,, \tag{3.69}$$

for all $F, G, H \in \mathcal{B}$. The Leibniz property, which is required for the Poisson bracket to generate a vector field, is built into the definition of functional derivative.

Upon inserting any functional of $\boldsymbol{\xi}$, say an observable o, into the Poisson bracket its evolution is determined by

$$\partial_t o = \{o, H\}\,, \tag{3.70}$$

where the Hamiltonian functional is the total energy of the system, where we rewrite (3.55) as follows:

$$H[\rho, \mathbf{m}, \sigma, \tilde{c}] = \int_\Omega e \;= \int_\Omega \frac{|\mathbf{m}|^2}{2\rho} + \rho u\left(\rho, \frac{\sigma}{\rho}, \frac{\tilde{c}}{\rho}\right). \tag{3.71}$$

Using the following functional derivatives:

$$\begin{aligned} &H_\rho = -|\mathbf{v}|^2/2 + u + p/\rho - sT - c\mu\,, \quad H_{\mathbf{m}} = \mathbf{v}\,, \\ &H_\sigma = T\,, \quad H_{\tilde{c}} = \mu\,, \end{aligned} \tag{3.72}$$

the bracket form of 3.70 gives the ideal two-phase flow system

$$\partial_t \mathbf{v} = \{\mathbf{v}, H\} = -\mathbf{v}\cdot\nabla\mathbf{v} - \nabla p/\rho\,, \tag{3.73}$$

$$\partial_t \rho = \{\rho, H\} = -\mathbf{v}\cdot\nabla\rho - \rho\,\nabla\cdot\mathbf{v}\,, \tag{3.74}$$

$$\partial_t \tilde{c} = \{\tilde{c}, H\} = -\mathbf{v}\cdot\nabla\tilde{c} - \tilde{c}\,\nabla\cdot\mathbf{v}\,, \tag{3.75}$$

$$\partial_t \sigma = \{\sigma, H\} = -\mathbf{v}\cdot\nabla\sigma - \sigma\,\nabla\cdot\mathbf{v}\,. \tag{3.76}$$

Equations (3.73)–(3.75) can also be written easily using , e.g., $\mathrm{D}\rho/\mathrm{D}t \coloneqq \partial\rho/\partial t + \mathbf{v}\cdot\nabla\rho$. These equations comprise the GE system.

Casimir invariants are special functionals $\mathfrak{C}$ that satisfy

$$\{F, \mathfrak{C}\} = 0 \qquad \forall F \in \mathcal{B}\,, \tag{3.77}$$

and thus are constants of motion for any Hamiltonian. From (3.68) we obtain the following equations that a Casimir functional $\mathfrak{C}$ must satisfy:

$$\nabla\cdot(\rho\,\mathfrak{C}_{\mathbf{m}}) = \nabla\cdot(\sigma\,\mathfrak{C}_{\mathbf{m}}) = \nabla\cdot(\tilde{c}\,\mathfrak{C}_{\mathbf{m}}) = 0\,, \tag{3.78}$$

and

$$m_j\nabla\mathfrak{C}_{m_j} + \partial_j(\mathbf{m}\,\mathfrak{C}_{m_j}) + \rho\,\nabla\mathfrak{C}_\rho + \sigma\,\nabla\mathfrak{C}_\sigma + \tilde{c}\,\nabla\mathfrak{C}_{\tilde{c}} = 0\,, \tag{3.79}$$

where we use the shorthand $\delta\mathfrak{C}/\delta\mathbf{m} \coloneqq \mathfrak{C}_{\mathbf{m}}$, $\delta\mathfrak{C}/\delta\rho \coloneqq \mathfrak{C}_\rho$, etc. and summation of

repeated indices is assumed. For the purpose at hand we assume $\mathfrak{C}$ is independent of $\mathbf{m}$, yielding the single condition

$$\rho\,\nabla\mathfrak{C}_\rho + \sigma\,\nabla\mathfrak{C}_\sigma + \tilde{c}\,\nabla\mathfrak{C}_{\tilde{c}} = 0\,. \tag{3.80}$$

Equation (3.80) is satisfied by

$$\mathfrak{C} = \int_\Omega \mathcal{C}(\rho, \sigma, \tilde{c}) \tag{3.81}$$

for any $\mathcal{C}$ that is Euler homogeneous of degree one, i.e., satisfies

$$\mathcal{C}(\lambda\rho, \lambda\sigma, \lambda\tilde{c}) = \lambda\,\mathcal{C}(\rho, \sigma, \tilde{c})\,. \tag{3.82}$$

The proof of this is straightforward.

To complete the third step of our algorithm, the entropy functional must be chosen from the set of Casimir invariants. Writing the Euler homogeneous integrand as

$$\mathcal{C}(\rho, \sigma, \tilde{c}) = \rho f(\sigma/\rho, \tilde{c}/\rho)$$

it is clear that

$$S = \int_\Omega \rho\, s = \int_\Omega \sigma \tag{3.83}$$

lies in our set of Casimirs. This quantity was first shown to be a Casimir for the ideal fluid in [Morrison, 1982] and used for the thermodynamically consistent Navier-Stokes metriplectic system in [Morrison, 1984a]. We note in passing, for other theories that might have a nontraditional dynamical equilibrium playing the role of thermodynamic equilibrium, one may wish to choose another Casimir.

3.3.3 METRIPLECTIC 4-BRACKET FOR THE GNS SYSTEM

To construct the metriplectic 4-bracket, we proceed as in Sec. 3.1 with the forms of M and Σ given by (3.6) and (3.7). Thus the determination of our system is complete when we make choices in (2.79) 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 (2.61):

$$\begin{aligned}
\mathbf{J}_\rho &= -L^{\rho\rho}\cdot\mathcal{L}^\rho_*(H_\rho) - L^{\rho\mathbf{m}}\colon\mathcal{L}^\mathbf{m}_*(H_\mathbf{m}) - L^{\rho\sigma}\cdot\mathcal{L}^\sigma_*(H_\sigma) - L^{\rho\tilde{c}}\cdot\mathcal{L}^{\tilde{c}}_*(H_{\tilde{c}})\,,\\
\bar{J}_\mathbf{m} &= -L^{\mathbf{m}\rho}\otimes\mathcal{L}^\rho_*(H_\rho) - L^{\mathbf{mm}}:\mathcal{L}^\mathbf{m}_*(H_\mathbf{m}) - L^{\mathbf{m}\sigma}\otimes\mathcal{L}^\sigma_*(H_\sigma) - L^{\mathbf{m}\tilde{c}}\otimes\mathcal{L}^{\tilde{c}}_*(H_{\tilde{c}})\,,\\
\mathbf{J}_c &= -L^{\tilde{c}\rho}\cdot\mathcal{L}^\rho_*(H_\rho) - L^{\tilde{c}\mathbf{m}}\colon\mathcal{L}^\mathbf{m}_*(H_\mathbf{m}) - L^{\tilde{c}\sigma}\cdot\mathcal{L}^\sigma_*(H_\sigma) - L^{\tilde{c}\tilde{c}}\cdot\mathcal{L}^{\tilde{c}}_*(H_{\tilde{c}})\,,\\
\mathbf{J}_s &= -L^{\sigma\rho}\cdot\mathcal{L}^\rho_*(H_\rho) - L^{\sigma\mathbf{m}}\colon\mathcal{L}^\mathbf{m}_*(H_\mathbf{m}) - L^{\sigma\sigma}\cdot\mathcal{L}^\sigma_*(H_\sigma) - L^{\sigma\tilde{c}}\cdot\mathcal{L}^{\tilde{c}}_*(H_{\tilde{c}})\,.
\end{aligned}\tag{3.84}$$

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

Now we specialize and show that the general expressions for the fluxes of (3.84) reduce to GNS. For example, if we choose $\mathcal{L}^{(\alpha)}_* = \nabla$, for all α, and H to be the expression of (3.71), then we obtain the GNS system using

$$H_\rho = -\frac{|\mathbf{m}|^2}{2\rho^2} + u + \frac{p}{\rho} - \frac{\sigma}{\rho}T - \frac{\tilde{c}}{\rho}\mu\,, \tag{3.85}$$

$$H_{\tilde{c}} = \mu\,, \tag{3.86}$$

$$H_\mathbf{m} = \mathbf{v}\,, \tag{3.87}$$

$$H_\sigma = T\,. \tag{3.88}$$

Upon setting all the $L^{\alpha\beta}$ to zero except

$$L^{\mathbf{mm}} = \bar{\bar{\Lambda}}\,,\quad L^{\sigma\sigma} = \frac{\bar{\kappa}}{T}\,,\quad \text{and}\quad L^{\tilde{c}\tilde{c}} = \bar{D}\,. \tag{3.89}$$

Equations (3.174) for the fluxes reduce to the known fluxes given in (3.58) - (3.62).

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

$$M(dF,dG) = F_\sigma G_\sigma\,, \tag{3.90}$$

$$\Sigma(dF,dG) = \nabla F_\mathbf{m} : \bar{\bar{\Lambda}} : \nabla G_\mathbf{m} + \nabla F_\sigma\cdot\frac{\bar{\kappa}}{T^2}\cdot\nabla G_\sigma + \nabla(F_{\tilde{c}})\cdot\frac{\bar{D}}{T}\cdot\nabla(G_{\tilde{c}})\,, \tag{3.91}$$

is

$$\begin{aligned}
(F,K;G,N) = \int_\Omega \frac{1}{T}\Big[\,&[K_\sigma\nabla F_\mathbf{m} - F_\sigma\nabla K_\mathbf{m}]:\bar{\bar{\Lambda}}:[N_\sigma\nabla G_\mathbf{m} - G_\sigma\nabla N_\mathbf{m}]\\
&+\frac{1}{T}\big[K_\sigma\nabla F_\sigma - F_\sigma\nabla K_\sigma\big]\cdot\bar{\kappa}\cdot\big[N_\sigma\nabla G_\sigma - G_\sigma\nabla N_\sigma\big]\\
&+\big[K_\sigma\nabla F_{\tilde{c}} - F_\sigma\nabla K_{\tilde{c}}\big]\cdot\bar{D}\cdot\big[N_\sigma\nabla G_{\tilde{c}} - G_\sigma\nabla N_{\tilde{c}}\big].
\end{aligned}\tag{3.92}$$

Upon insertion of H as given by (3.71) and S from the set of Casimirs of Sec.3.3.2 to be as in (3.83), the dynamics is given by

$$\partial_t \xi^\alpha = \{\xi^\alpha, H\} + (\xi^\alpha, H; S, H)\,. \tag{3.93}$$

Using $H_{\mathbf{m}} = \mathbf{v}$, $H_\sigma = T$, and $S_\sigma = 1$, the following GNS system is produced:

$$\begin{aligned}
\partial_t \mathbf{v} &= \{\mathbf{v}, H\} + (\mathbf{v}, H; S, H) \\
&= -\mathbf{v}\cdot\nabla\mathbf{v} - \nabla p/\rho + \frac{1}{\rho}\nabla\cdot(\bar{\bar{\Lambda}} : \nabla\mathbf{v})\,, && (3.94)\\
\partial_t \rho &= \{\rho, H\} + (\rho, H; S, H) \\
&= -\mathbf{v}\cdot\nabla\rho - \rho\,\nabla\cdot\mathbf{v}\,, && (3.95)\\
\partial_t \tilde{c} &= \{\tilde{c}, H\} + (\tilde{c}, H; S, H) \\
&= -\mathbf{v}\cdot\nabla\tilde{c} - \tilde{c}\,\nabla\cdot\mathbf{v} + \nabla\cdot(\bar{D}\cdot\nabla\mu)\,, && (3.96)\\
\partial_t \sigma &= \{\sigma, H\} + (\sigma, H; S, H) \\
&= -\mathbf{v}\cdot\nabla\sigma - \sigma\,\nabla\cdot\mathbf{v} + \nabla\cdot\left(\frac{\bar{\kappa}}{T}\cdot\nabla T\right) + \frac{1}{T^2}\nabla T\cdot\bar{\kappa}\cdot\nabla T \\
&\qquad + \frac{1}{T}\nabla\mathbf{v} : \bar{\bar{\Lambda}} : \nabla\mathbf{v} + \frac{1}{T}\nabla\mu\cdot\bar{D}\cdot\nabla\mu\,. && (3.97)
\end{aligned}$$

By construction we automatically have energy conservation, i.e., for (3.71) $\dot{H} = 0$, and entropy production

$$\begin{aligned}
\dot{S} &= (S, H; S, H) \\
&= \int_\Omega \frac{1}{T}\left[\nabla\mathbf{v} : \bar{\bar{\Lambda}} : \nabla\mathbf{v} + \frac{1}{T}\nabla T\cdot\bar{\kappa}\cdot\nabla T + \nabla\mu\cdot\bar{D}\cdot\nabla\mu\right] \geq 0\,. && (3.98)
\end{aligned}$$

3.3.4 METRIPLECTIC 2-BRACKET FOR GNS SYSTEM

To further identify the meaning of $L^{\alpha\beta}$ we revisit the thermodynamics of (3.65), in light of the choice of the variables $\boldsymbol{\xi} = (\rho, \mathbf{m}, \tilde{c}, e)$. Thus, we rewrite the thermodynamic relation 3.65 upon changing variables,

$$T\mathrm{d}\sigma = \mathrm{d}e - \mathbf{v}\cdot\mathrm{d}\mathbf{m} - \mu\mathrm{d}\tilde{c} - g\mathrm{d}\rho\,, \tag{3.99}$$

where e is the energy density of (3.64) and g is a modified specific Gibbs free energy, viz.

$$g := u - Ts + p/\rho - \mu c - |\mathbf{v}|^2/2\,. \tag{3.100}$$

We have assumed in (3.53) that there is no flux associated with ρ, i.e., in CHNS chemical reactions and/or particle creation and annihilation are ignored. Thus, the phase space for the thermodynamics is smaller than that for the Hamiltonian dynamics, because the variable ρ as seen e.g. in (3.95) has no dissipative terms. This leads us to focus on the thermodynamic variables $(\mathbf{m}, \tilde{c}, e)$ and (3.99) reduces to

$$T\mathrm{d}\sigma = \mathrm{d}e - \mathbf{v}\cdot\mathrm{d}\mathbf{m} - \mu\mathrm{d}\tilde{c}\,. \tag{3.101}$$

Comparison of (2.53) and (3.66) suggests we require the affinities associated with $\mathbf{m}$, $\tilde{c}$ and e. The conventional choices for these affinities are $\nabla(1/T)$, $\nabla(-\mathbf{v}/T)$, and $\nabla(-\mu/T)$, respectively [de Groot and Mazur, 1962]. However, examination of (3.63) or (3.98) suggests using instead ∇T, $\nabla\mathbf{v}$, and $\nabla\mu$, as was done in Coquinot and Morrison [2020b].

The relationship between the flux-affinity relations in terms of these two choices of bases are given by the following:

$$\begin{aligned}
\bar{J}_{\mathbf{m}} &= L_{\mathbf{m}e}\cdot\nabla\left(\frac{1}{T}\right) + L_{\mathbf{mm}} : \nabla\left(\frac{-\mathbf{v}}{T}\right) + L_{\mathbf{m}\tilde{c}}\cdot\nabla\left(\frac{-\mu}{T}\right) \\
&= -\bar{\bar{\Lambda}} : \nabla\mathbf{v}\,, \qquad (3.102)\\
\mathbf{J}_e &= L_{ee}\cdot\nabla\left(\frac{1}{T}\right) + L_{e\mathbf{m}} : \nabla\left(\frac{-\mathbf{v}}{T}\right) + L_{e\tilde{c}}\cdot\nabla\left(\frac{-\mu}{T}\right) \\
&= -\mathbf{v}\cdot(\bar{\bar{\Lambda}} : \nabla\mathbf{v}) - \bar{\kappa}\cdot\nabla T - \mu\bar{D}\cdot\nabla\mu\,, \qquad (3.103)\\
\mathbf{J}_{\tilde{c}} &= L_{\tilde{c}e}\cdot\nabla\left(\frac{1}{T}\right) + L_{\tilde{c}\mathbf{m}} : \nabla\left(\frac{-\mathbf{v}}{T}\right) + L_{\tilde{c}\tilde{c}}\cdot\nabla\left(\frac{-\mu}{T}\right) \\
&= -\bar{D}\cdot\nabla\mu\,. \qquad (3.104)
\end{aligned}$$

Recall $\bar{J}_{\mathbf{m}}$ is a 2-tensor, thus $L_{\mathbf{m}e} = L_{e\mathbf{m}}$ is a 3-tensor, $L_{\mathbf{mm}}$ is a 4-tensor, and $L_{\mathbf{m}\tilde{c}} = L_{\tilde{c}\mathbf{m}}$ is a 3-tensor. Since $\mathbf{J}_e$ and $\mathbf{J}_{\tilde{c}}$ are vectors, $L_{ee}, L_{e\tilde{c}} = L_{\tilde{c}e}$, and $L_{\tilde{c}\tilde{c}}$ are 2-tensors. From (3.102), (3.103), and (3.104), we identify the components of $L_{\alpha\beta}$ as follows:

$$\begin{aligned}
&L_{\mathbf{m}e} = T\bar{\bar{\Lambda}}\cdot\mathbf{v}\,, \quad L_{\mathbf{mm}} = T\bar{\bar{\Lambda}}\,, \quad L_{\mathbf{m}\tilde{c}} = 0\,, \quad L_{e\tilde{c}} = T\mu\bar{D}\,,\\
&L_{ee} = T^2\bar{\kappa} + T\mathbf{v}\cdot\bar{\bar{\Lambda}}\cdot\mathbf{v} + T\mu^2\bar{D}\,, \quad L_{\tilde{c}\tilde{c}} = T\bar{D}\,.
\end{aligned} \tag{3.105}$$

The metriplectic 2-bracket in terms of the ξ-variables is given by

$$\begin{aligned}(F,G) = \int_\Omega T \Big[& \nabla F_e \cdot (T\bar{\kappa} + \mathbf{v}\cdot\bar{\bar{\Lambda}}\cdot\mathbf{v} + \mu^2\bar{D})\cdot\nabla G_e \\ & + \nabla F_{\mathbf{m}} : \bar{\bar{\Lambda}} : \nabla G_{\mathbf{m}} + \nabla F_{\tilde{c}}\cdot\bar{D}\cdot\nabla G_{\tilde{c}} \\ & + \nabla F_e\cdot(\bar{\bar{\Lambda}}\cdot\mathbf{v}) : \nabla G_{\mathbf{m}} + \nabla G_e\cdot(\bar{\bar{\Lambda}}\cdot\mathbf{v}) : \nabla F_{\mathbf{m}} \\ & + \mu\,\nabla F_e\cdot\bar{D}\cdot\nabla G_{\tilde{c}} + \mu\,\nabla G_e\cdot\bar{D}\cdot\nabla F_{\tilde{c}} \Big]. \end{aligned} \tag{3.106}$$

Upon writing

$$S = \int_\Omega \sigma(\rho, e, \tilde{c}, \mathbf{m}) \tag{3.107}$$

and using standard thermodynamic manipulations we obtain

$$S_e = 1/T\,, \quad S_{\mathbf{m}} = -\mathbf{v}/T\,, \quad \text{and} \quad S_{\tilde{c}} = -\mu/T\,. \tag{3.108}$$

Inserting these into (o,S) using the 2-bracket of (3.106) yields the dissipative terms of (3.94), (3.96), and with the manipulations of transforming from e to σ, those of the entropy equation (3.97). By direct calculation, as well as by construction, we obtain $(H,S)=0$ and $\dot{S} = (S,S) \geq 0$ which reproduces (3.98).

To close the circle we transform the bracket of (3.106) in terms of the variables $(\rho, \mathbf{m}, \tilde{c}, e)$ to one in terms of $(\rho, \mathbf{m}, \tilde{c}, \sigma)$ via the following chain rule formulas:

$$\begin{aligned} G_e \to G_\sigma/T, \qquad & G_{\mathbf{m}} \to G_{\mathbf{m}} - \mathbf{v}\,G_\sigma/T\,, \\ G_{\tilde{c}} \to G_{\tilde{c}} - \mu\,G_\sigma/T\,. & \end{aligned} \tag{3.109}$$

This calculation gives precisely the 2-bracket that comes from the 4-bracket (3.92)

$$(F,G) = (F,G)_H = (F,H;G,H). \tag{3.110}$$

3.4 FROM GNS TO CAHN-HILLIARD-NAVIER-STOKES

Now we apply the UT-algorithm to obtain the Cahn-Hilliard-Navier-Stokes system (CHNS) which allows for diffuse-interfaces. We follow the steps in order, just as in Sec.3.3. However, here we have the additional step of aligning the desired entropy functional with the Poisson bracket, so that it is indeed a Casimir invariant.

3.4.1 HAMILTONIAN AND ENTROPY FUNCTIONAL FORMS

The phenomenon of material transport along an interface is known as the Marangoni effect. The presence of a surface tension gradient naturally induces the migration of particles, moving from regions of low tension to those of high tension. This gradient can be triggered by a concentration gradient (or also a temperature gradient). In two-phase theory the interface between phases is regarded as being diffuse. According to the work of Taylor and Cahn [1998], one can model the diffuse interface by a single order parameter, say ϕ and with a free energy functional,

$$\mathfrak{F} = \int_{\Omega} \frac{\epsilon}{2} \Gamma^2(\nabla\phi) + \frac{1}{\epsilon} V(\phi)\,, \tag{3.111}$$

with Γ being a homogeneous function of degree one, further details on this will be provided later. Here V can be any non-negative function that equals zero at $\phi = \pm 1$ and ϵ is a small parameter that goes to zero in the sharp-interface limit. We choose the order parameter ϕ to be the concentration.

In the isotropic surface energy case Guo and Lin [2015] develop a phase-field model for two-phase flow, which is thermodynamically consistent. The modeling based on a non-classical choice of energy and entropy, given respectively by

$$H_{GL} = \int_{\Omega} \frac{\rho}{2} |\mathbf{v}|^2 + \rho u(\rho, s, c) + \frac{\rho}{2} \lambda_u |\nabla c|^2\,, \tag{3.112}$$

$$S_{GL} = \int_{\Omega} \rho s + \frac{\rho}{2} \lambda_s |\nabla c|^2\,, \tag{3.113}$$

where u and s stand for the classical specific internal energy and entropy, respectively, while the coefficients λ_s and λ_u are constant parameters.

Alternatively, Anderson et al. [2000] propose a model of phase-field of solidification with convection, the model permits the interface to have an anisotropic surface energy. The choice of energy and entropy are given by

$$H_{AMW} = \int_{\Omega} \frac{\rho}{2} |\mathbf{v}|^2 + \rho u(\rho, s, c) + \frac{\epsilon_E^2}{2} \Gamma^2(\nabla c)\,, \tag{3.114}$$

$$S_{AMW} = \int_{\Omega} \rho s - \frac{\epsilon_S^2}{2} \Gamma^2(\nabla c)\,, \tag{3.115}$$

where the coefficients ϵ_S and ϵ_E are assumed to be constant and Γ is a homogeneous

function of degree one that takes a vector to a real number.

In this section, we explore a choice of energy and entropy functionals, from which the previously mentioned choices are special cases, and we consider the associated free energy functional, viz.

$$H^a = \int_\Omega \frac{\rho}{2}|\mathbf{v}|^2 + \rho u + \frac{\rho^a}{2}\lambda_u \Gamma^2(\nabla c) =: \int_\Omega e^a_{\text{Total}}\,, \tag{3.116}$$

$$S^a = \int_\Omega \rho s + \frac{\rho^a}{2}\lambda_s \Gamma^2(\nabla c) =: \int_\Omega \sigma^a_{\text{Total}}\,, \tag{3.117}$$

$$\mathfrak{F}^a = \int_\Omega \rho f + \frac{\rho^a}{2}\lambda_f(T) \Gamma^2(\nabla c)\,, \tag{3.118}$$

where u, s and f stand for the classical specific internal energy, entropy, and free energy, respectively, the coefficients λ_s and λ_u are constant parameters, and $\lambda_f(T)$ is a parameter depending on the temperature that will lead to anisotropic surface energy effects. He have defined the total densities e^a_{Total} and σ^a_{Total} for later use. The parameter a takes on two values: $a = 0$ reduces (3.116) and (3.117) to the expressions of Anderson et al. [2000], where we set $\epsilon_E^2 = \lambda_u$ and $\epsilon_S^2 = -\lambda_s$, while for $a = 1$ they reduce to those used by Guo and Lin [2015] provided the choice of an isotropic surface energy is assumed, viz., $\Gamma(\nabla c) = |\nabla c|$. Thus, as is clear from (3.117), (3.116), and (3.118) that the dimensions of λ_f, λ_s, and λ_u are either specific or volumetric depending on the case. As usual, we have the thermodynamic relation

$$f = u - Ts\,, \tag{3.119}$$

which allows us to assume the relationship between the coefficients

$$\lambda_f(T) = \lambda_u - T\lambda_s \quad \text{and} \quad \frac{\mathrm{d}\lambda_f(T)}{\mathrm{d}T} = -\lambda_s\,. \tag{3.120}$$

To summarize, our expressions (3.116) and (3.117) generalize the model studied by Guo and Lin [2015] by including Γ, which accounts for anisotropic surface energy effects, while our expressions generalize the model of Anderson et al. [2000] by including the factors of ρ in the integrands making all quantities in the integrands specific quantities multiplied by the density, giving rise to more general sources of energy.

Because Γ is a homogeneous function of degree unity,

$$\Gamma(\lambda \mathbf{p}) = \lambda \Gamma(\mathbf{p}) \text{ for all } \lambda > 0\,. \tag{3.121}$$

Differentiating (3.121) with respect to λ and then setting $\lambda = 1$ yields the fundamental relation

$$\Gamma(\mathbf{p}) = \mathbf{p} \cdot \boldsymbol{\zeta} \coloneqq p_j \frac{\partial \Gamma(\mathbf{p})}{\partial p_j} \,. \tag{3.122}$$

Then, differentiating (3.122) gives a second well-known relation,

$$\frac{\partial \Gamma}{\partial p_i} = \frac{\partial}{\partial p_i}(\boldsymbol{\zeta} \cdot \mathbf{p}) = \xi_i + \frac{\partial^2 \Gamma}{\partial p_i \partial p_j} p_j = \xi_i \,, \tag{3.123}$$

where evidently p_j must be a null eigenvector of the matrix $\partial^2\Gamma/\partial p_i \partial p_j$. Henceforth we will assume the argument of Γ to be ∇c. For the case of isotropic surface energy, where $\Gamma(\nabla c) = |\nabla c|$, the associated homogeneous function of degree zero is given by

$$\boldsymbol{\zeta} = \frac{\nabla c}{|\nabla c|} \,. \tag{3.124}$$

From (3.118) we can obtain a generalized chemical potential

$$\begin{aligned} \mu^a_\Gamma \coloneqq \frac{\delta \mathfrak{F}^a}{\delta \tilde{c}} &= \rho \frac{\partial u}{\partial \tilde{c}} - \nabla \cdot (\lambda_f \rho^a \Gamma \nabla c) \\ &= \mu - \frac{1}{\rho} \nabla \cdot (\lambda_f \rho^a \Gamma \boldsymbol{\zeta}) \,, \end{aligned} \tag{3.125}$$

where recall $\tilde{c} = \rho c$. For the case of isotropic surface energy, this becomes

$$\mu^a_{|\nabla c|} = \mu - \frac{1}{\rho} \nabla \cdot (\lambda_f \rho^a \nabla c) \,. \tag{3.126}$$

Upon setting $a = 1$ [the case of Guo and Lin, 2015], this reduces to

$$\mu^1_{|\nabla c|} = \mu - \frac{1}{\rho} \nabla \cdot (\lambda_f \rho \, \nabla c) \,, \tag{3.127}$$

an expression that differs from that in Guo and Lin [2015] unless $\lambda_f \rho$ is constant. If this is the case and we choose a classical $\mu = c^3 - c$, corresponding to the quartic Laudau potential, we obtain

$$\mu_{CH} = c^3 - c - \lambda_f \nabla^2 c \,, \tag{3.128}$$

also one can choose a free energy corresponding to Logarithm potential

$$\mu = \frac{\lambda_1}{2}(1 - c^2) + \frac{\lambda_2}{2} \left[(1 + c) \ln \frac{(1 + c)}{2} + (1 - c) \ln \frac{(1 - c)}{2} \right]$$

where $0 < \lambda_2 < \lambda_1$. the chemical potential of Cahn and Hilliard who indeed make these assumptions [cf. page 267 of Cahn and Hilliard, 1958]. For $\alpha = 0$ [the case of Anderson et al., 2000], we have

$$\mu_\Gamma^0 = \mu - \frac{1}{\rho}\nabla \cdot (\lambda_f \, \Gamma \boldsymbol{\zeta}) \,, \tag{3.129}$$

which allows for the weighted mean curvature effects of anisotropy.

Maintaining the same set of dynamical variables as in (3.67) (or an equivalent set) and making the choices of energy and entropy functionals of (3.116) and (3.117), we have completed the first two steps of the UT-algorithm.

3.4.2 NONCANONICAL POISSON BRACKET OF THE CAHN-HILLIARD-EULER SYSTEM

To complete the next step of the algorithm, the third step, we need to manufacture a bracket that has (3.117) as a Casimir invariant. We do this by starting from the bracket of (3.68) in terms of the original variables $\boldsymbol{\xi} = \{\mathbf{m}, \rho, \tilde{c}, \sigma\}$ and then transforming it to a new set of dynamical variables

$$\hat{\boldsymbol{\xi}}^a \coloneqq \{\hat{\mathbf{m}}, \hat{\rho}, \hat{\tilde{c}}, \hat{\sigma}^a\} \,, \tag{3.130}$$

giving the same bracket in terms of new coordinates. We have included the superscript a because in effect we have two sets of coordinates, corresponding to the desired entropies of (3.117) for $a = 0$ and $a = 1$. To distinguish the old from the new, we write the bracket in the transformed variables as $\{\hat{F}, \hat{G}\}^a$. Because of coordinate invariance, $\{C, F\} = \{C^a, \hat{F}\}^a = 0$, where $F[\boldsymbol{\xi}] = \hat{F}[\hat{\boldsymbol{\xi}}^a]$ is any functional written in one or the other coordinates. The Casimir $S = \int_\Omega \sigma$ in our original coordinates is transformed into a different form in the new coordinates. Specifically, we change the variables as follows:

$$\begin{aligned} &\mathbf{m} = \hat{\mathbf{m}} \,, \quad \rho = \hat{\rho} \,, \quad \tilde{c} = \hat{\tilde{c}} \,, \\ &\sigma = \hat{\sigma}^a + \frac{\hat{\rho}^a}{2}\lambda_s \Gamma^2 (\nabla \hat{c}) \,, \end{aligned} \tag{3.131}$$

where $\hat{\tilde{c}} = \hat{\rho}\hat{c}$. Consequently, the entropy S in the old coordinates written in terms of the new coordinates will, by design, become the following Casimir for the Poisson

bracket in the new coordinates:

$$\hat{S}^a = \int_\Omega \hat{\sigma}^a + \frac{\hat{\rho}^a}{2}\lambda_s\Gamma^2(\nabla\hat{c})\,. \tag{3.132}$$

Thus we have manufactured a bracket with the entropy expression of (3.117) as a Casimir.

Transformation of the Poisson bracket (3.68) requires use of the functional chain rule. For convenience we use

$$\hat{\sigma}^a = \sigma - \frac{\rho^a}{2}\lambda_s\Gamma^2(\nabla c) \tag{3.133}$$

and consider the variation of any functional of the new variables. Thus we use $\delta\rho = \delta\hat{\rho}$, $\delta\mathbf{m} = \delta\hat{\mathbf{m}}$, $\delta\tilde{c} = \delta\hat{\tilde{c}}$, and for the entropy variable

$$\begin{aligned}\delta\hat{\sigma}^a &= \delta\sigma - \frac{1}{2}a\rho^{a-1}\lambda_s\Gamma^2(\nabla c)\delta\rho - \rho^a\lambda_s\Gamma\boldsymbol{\zeta}\cdot\nabla\delta\left(\frac{\tilde{c}}{\rho}\right)\\ &= \delta\sigma - \frac{1}{2}a\rho^{a-1}\lambda_s\Gamma^2(\nabla c)\delta\rho - \rho^a\lambda_s\Gamma\boldsymbol{\zeta}\cdot\nabla\left(\frac{\delta\tilde{c}}{\rho}\right) + \rho^a\lambda_s\Gamma\boldsymbol{\zeta}\cdot\nabla\left(\frac{\tilde{c}}{\rho^2}\delta\rho\right)\,,\end{aligned} \tag{3.134}$$

where use has been made of (3.123). Now let F be an arbitrary functional of the original variables and $\hat{F}$ the same functional in terms of the new variables. Thus,

$$\int_\Omega \hat{F}_{\hat{\mathbf{m}}}\cdot\,\delta\hat{\mathbf{m}} + \hat{F}_{\hat{\rho}}\,\delta\hat{\rho} + \hat{F}_{\hat{\sigma}^a}\,\delta\hat{\sigma}^a + \hat{F}_{\hat{\tilde{c}}}\,\delta\hat{\tilde{c}} = \int_\Omega F_{\mathbf{m}}\cdot\delta\mathbf{m} + F_\rho\,\delta\rho + F_\sigma\,\delta\sigma + F_{\tilde{c}}\,\delta\tilde{c}\,.$$

Note, no sum over a is to be done. By identification of terms we obtain

$$\begin{aligned}&F_{\mathbf{m}} = \hat{F}_{\hat{\mathbf{m}}}\,,\quad F_\sigma = \hat{F}_{\hat{\sigma}_a}\,,\\ &F_\rho = \hat{F}_{\hat{\rho}} - \frac{a}{2}\hat{\rho}^{a-1}\lambda_s\Gamma^2\,\hat{F}_{\hat{\sigma}^a} - \frac{\hat{\tilde{c}}}{\hat{\rho}^2}\,\nabla\cdot\left(\hat{\rho}^a\lambda_s\Gamma\boldsymbol{\zeta}\,\hat{F}_{\hat{\sigma}^a}\right)\,,\\ &F_{\tilde{c}} = \hat{F}_{\hat{\tilde{c}}} + \frac{1}{\hat{\rho}}\nabla\cdot\left(\hat{\rho}^a\lambda_s\Gamma\boldsymbol{\zeta}\hat{F}_{\hat{\sigma}^a}\right)\,.\end{aligned} \tag{3.135}$$

The transformed Poisson bracket is obtained by inserting the expressions of (3.135) into (3.68), writing it entirely in terms of the hat variables. Upon doing this and then dropping the hats, we get for any functionals F and G the following Poisson

bracket:

$$\begin{aligned}\{F,G\}^a = -\int_\Omega \mathbf{m}\cdot\Big[F_{\mathbf{m}}\cdot\nabla G_{\mathbf{m}} - G_{\mathbf{m}}\cdot\nabla F_{\mathbf{m}}\Big] \\ + \rho\Big[F_{\mathbf{m}}\cdot\nabla\big(G_\rho - a\rho^{a-1}\lambda_s\Gamma^2 G_{\sigma^a}/2 - \tilde{c}\,\nabla\cdot(\rho^a\lambda_s\Gamma\boldsymbol{\zeta}G_{\sigma^a})/\rho^2\big) \\ - G_{\mathbf{m}}\cdot\nabla\big(F_\rho - a\rho^{a-1}\lambda_s\Gamma^2 F_{\sigma^a}/2 - \tilde{c}\,\nabla\cdot(\rho^a\lambda_s\Gamma\boldsymbol{\zeta}F_{\sigma^a})/\rho^2\big)\Big] \\ + \big(\sigma^a + \rho^a\lambda_s\Gamma^2/2\big)\Big[F_{\mathbf{m}}\cdot\nabla G_{\sigma^a} - G_{\mathbf{m}}\cdot\nabla F_{\sigma^a}\Big] \\ + \tilde{c}\Big[F_{\mathbf{m}}\cdot\nabla\left(G_{\tilde{c}} + \nabla\cdot(\rho^a\lambda_s\Gamma\boldsymbol{\zeta}G_{\sigma^a})/\rho\right) \\ - G_{\mathbf{m}}\cdot\nabla\left(F_{\tilde{c}} + \nabla\cdot(\rho^a\lambda_s\Gamma\boldsymbol{\zeta}F_{\sigma^a})/\rho\right)\Big]. \end{aligned} \tag{3.136}$$

This bracket is clearly bilinear and skew-symmetric. Because it was derived from the bracket 3.68 by a change of variables, satisfaction of the Jacobi identity is assured. We note, as before, strong boundary conditions are assumed such that all integrations by parts produce vanishing boundary terms.

Thus we have completed the third part of our algorithm, the construction of a Poisson bracket that has entropy functional of (3.117) in the set of its Casimir invariants. Recall the integrand of the entropy is given by

$$\sigma^a_{\text{Total}} \coloneqq \sigma^a + \frac{\rho^a}{2}\lambda_s\Gamma^2(\nabla c)\,; \tag{3.137}$$

so we find

$$\begin{aligned}\frac{\delta S^a}{\delta\sigma^a} = 1\,, \quad \frac{\delta S^a}{\delta\tilde{c}} = -\frac{1}{\rho}\nabla\cdot(\rho^a\lambda_s\Gamma\boldsymbol{\zeta}) \\ \frac{\delta S^a}{\delta\rho} = \frac{a}{2}\rho^{a-1}\lambda_s\Gamma^2 + \frac{\tilde{c}}{\rho^2}\nabla\cdot(\rho^a\lambda_s\Gamma\boldsymbol{\zeta})\,. \end{aligned} \tag{3.138}$$

Using (3.138) one can easily check that $\{F, S^a\} = 0$ for all F, which by construction had to be the case. Now we are free to choose any Hamiltonian we desire in (3.136) to obtain the evolution of any observable o as follows:

$$\partial_t o = \{o, H^a\}^a\,, \tag{3.139}$$

In Sec.3.4.1 we proposed the Hamiltonian functional of (3.116), which we rewrite as

follows in order to make all arguments clear:

$$H^a[\rho, \mathbf{m}, \sigma, \tilde{c}] = \int_\Omega \frac{|\mathbf{m}|^2}{2\rho} + \rho u\left(\rho, \frac{\sigma^a}{\rho}, \frac{\tilde{c}}{\rho}\right) + \frac{\rho^a}{2}\lambda_u \Gamma^2 \left(\nabla\left(\frac{\tilde{c}}{\rho}\right)\right) . \tag{3.140}$$

Using the functional derivatives of this Hamiltonian,

$$\begin{aligned} H^a_{\mathbf{m}} &= \mathbf{v}, \quad H_{\sigma^a} = T\,, \\ H^a_\rho &= -|\mathbf{v}|^2/2 + u + p/\rho - sT - c\mu + a\rho^{a-1}\lambda_u\Gamma^2/2 + c\,\nabla\cdot(\rho^a\lambda_u\Gamma\boldsymbol{\zeta})/\rho\,, \\ H^a_{\tilde{c}} &= \mu - \nabla\cdot(\rho^a\lambda_u\Gamma\boldsymbol{\zeta})/\rho\,, \end{aligned} \tag{3.141}$$

in the bracket (3.136) gives the equations of motion in the form of (3.139). At this point we could write this out and display a general system of equations that includes both cases, but we choose to consider them separately because the general system is unwieldy and not particularly perspicuous.

Let us first consider the simplified version of our derived Poisson bracket for the case $a = 1$, which is as follows:

$$\begin{aligned} \{F, G\}^1 = -\int_\Omega \mathbf{m}\cdot\big[F_{\mathbf{m}}\cdot\nabla G_{\mathbf{m}} - G_{\mathbf{m}}\cdot\nabla F_{\mathbf{m}}\big] \\ + \rho\big[F_{\mathbf{m}}\cdot\nabla G_\rho - G_{\mathbf{m}}\cdot\nabla F_\rho\big] \\ - \lambda_s\big[F_{\mathbf{m}}\cdot\nabla\cdot(\rho G_{\sigma^1}\Gamma\boldsymbol{\zeta}\otimes\nabla c) - G_{\mathbf{m}}\cdot\nabla\cdot(\rho F_{\sigma^1}\Gamma\boldsymbol{\zeta}\otimes\nabla c)\big] \\ + \sigma^1\left[F_{\mathbf{m}}\cdot\nabla G_{\sigma^1} - G_{\mathbf{m}}\cdot\nabla F_{\sigma^1}\right] \\ + \tilde{c}\left[F_{\mathbf{m}}\cdot\nabla G_{\tilde{c}} - G_{\mathbf{m}}\cdot\nabla F_{\tilde{c}}\right]\,, \end{aligned} \tag{3.142}$$

where $\otimes$ denotes tensor product of two vectors and consistent with our convention we have

$$\nabla\cdot(\mathbf{u}\otimes\mathbf{v}) = (\nabla\cdot\mathbf{u})\mathbf{v} + \mathbf{u}\cdot\nabla\mathbf{v}\,.$$

Using (3.141), the bracket form of (3.139) gives the ideal diffuse two-phase flow system

$$\partial_t\mathbf{v} = \{\mathbf{v}, H^1\}^1 = -\mathbf{v}\cdot\nabla\mathbf{v} - \frac{1}{\rho}\nabla\cdot(p\bar{I} + \rho\lambda_f\Gamma\boldsymbol{\zeta}\otimes\nabla c)\,, \tag{3.143}$$

$$\partial_t\rho = \{\rho, H^1\}^1 = -\mathbf{v}\cdot\nabla\rho - \rho\,\nabla\cdot\mathbf{v}\,, \tag{3.144}$$

$$\partial_t\tilde{c} = \{\tilde{c}, H^1\}^1 = -\mathbf{v}\cdot\nabla\tilde{c} - \tilde{c}\,\nabla\cdot\mathbf{v}\,, \tag{3.145}$$

$$\partial_t\sigma^1_{\text{Total}} = \{\sigma^1_{\text{Total}}, H^1\}^1 = -\mathbf{v}\cdot\nabla\sigma^1_{\text{Total}} - \sigma^1_{\text{Total}}\,\nabla\cdot\mathbf{v}\,, \tag{3.146}$$

where $\bar{I}$ is the unit tensor. Observe in (3.146) we have chosen the observable σ^1_{Total}

instead of σ^1, in order to demonstrate its conservation.

Similarly, for the case where $a = 0$, the Poisson bracket has the following form:

$$\begin{aligned}\{F, G\}^0 = -\int_\Omega \mathbf{m} \cdot & \left[F_{\mathbf{m}} \cdot \nabla G_{\mathbf{m}} - G_{\mathbf{m}} \cdot \nabla F_{\mathbf{m}}\right] \\ & + \rho\left[F_{\mathbf{m}} \cdot \nabla G_\rho - G_{\mathbf{m}} \cdot \nabla F_\rho\right] \\ & - \lambda_s\left[F_{\mathbf{m}} \cdot \nabla \cdot (G_{\sigma^0}\Gamma\boldsymbol{\zeta} \otimes \nabla c) - G_{\mathbf{m}} \cdot \nabla \cdot (F_{\sigma^0}\Gamma\boldsymbol{\zeta} \otimes \nabla c)\right] \\ & + \lambda_s\left[F_{\mathbf{m}} \cdot \nabla\left(\Gamma^2 G_{\sigma^0}\right) - G_{\mathbf{m}} \cdot \nabla\left(\Gamma^2 F_{\sigma^0}\right)\right]/2 \\ & + \sigma^0\left[F_{\mathbf{m}} \cdot \nabla G_{\sigma^0} - G_{\mathbf{m}} \cdot \nabla F_{\sigma^0}\right] \\ & + \tilde{c}\left[F_{\mathbf{m}} \cdot \nabla G_{\tilde{c}} - G_{\mathbf{m}} \cdot \nabla F_{\tilde{c}}\right] . \end{aligned} \tag{3.147}$$

Same as above, using (3.141), the ideal diffuse two-phase flow system is produced

$$\partial_t \mathbf{v} = \{\mathbf{v}, H^0\}^0 = -\mathbf{v} \cdot \nabla \mathbf{v} - \frac{1}{\rho}\nabla \cdot \left[\left(p - \lambda_f \Gamma^2/2\right)\bar{I} + \lambda_f \Gamma \boldsymbol{\zeta} \otimes \nabla c\right], \tag{3.148}$$

$$\partial_t \rho = \{\rho, H^0\}^0 = -\mathbf{v} \cdot \nabla \rho - \rho\, \nabla \cdot \mathbf{v}\,, \tag{3.149}$$

$$\partial_t \tilde{c} = \{\tilde{c}, H^0\}^0 = -\mathbf{v} \cdot \nabla \tilde{c} - \tilde{c}\, \nabla \cdot \mathbf{v}\,, \tag{3.150}$$

$$\partial_t \sigma^0_{\text{Total}} = \{\sigma^0_{\text{Total}}, H^0\}^0 = -\mathbf{v} \cdot \nabla \sigma^0_{\text{Total}} - \sigma^0_{\text{Total}}\, \nabla \cdot \mathbf{v}\,. \tag{3.151}$$

where recall from (3.122), $\boldsymbol{\zeta} = \partial\Gamma/\partial\mathbf{p}$.

Let us now comment on these two Hamiltonian systems. By construction both the $a = 1$ and $a = 0$ systems conserve their Hamiltonians and entropies, as given by (3.117) and (3.116) with $a = 1$ and $a = 0$, respectively. Both systems have momentum equations containing a term describing anisotropic surface energy (capillary) effects. The $a = 0$ system of (3.148)–(3.151) is identical to the ideal limit of that given in the work of Anderson et al. [2000]. Upon choosing $\Gamma(\nabla c) = |\nabla c|$, the $a = 1$ system of (3.143)–(3.146) should correspond to the ideal limit of that of Guo and Lin [2015], but it does not. In fact the system of Guo and Lin [2015] in this limit does not conserve energy. Moreover, the capillary effect in their momentum equation (equation (3.40)), which should be replaced by (3.143) with $\Gamma(\nabla c) = |\nabla c|$, vanishes in the one-dimensional limit. Since such surface effects are determined by mean or weighted mean curvature [Taylor, 1992], it is clear that this is physically untenable. Fortunately, our method provides a simple fix to their equations, while showing how to generalize them to include anisotropic surface effects.

3.4.3 METRIPLECTIC 4-BRACKET FOR THE CAHN-HILLIARD-NAVIER-STOKES SYSTEM

Now we turn to the 4th and final step of the UT-algorithm. As we did in the construction of noncanonical Poisson Bracket, we change variables and use the obtained 4-bracket of GNS of Sec.3.3.3. The transformed metriplectic 4-bracket is obtained by inserting the expressions of (3.135) into (3.92), we get

$$
\begin{aligned}
(F,K;G,N)^a = \int_\Omega \frac{1}{T}\Big[& [K_{\sigma^a}\nabla F_{\mathbf{m}} - F_{\sigma^a}\nabla K_{\mathbf{m}}] : \bar{\bar{\Lambda}} : [N_{\sigma^a}\nabla G_{\mathbf{m}} - G_{\sigma^a}\nabla N_{\mathbf{m}}] \\
& + \frac{1}{T}\big[K_{\sigma^a}\nabla F_{\sigma^a} - F_{\sigma^a}\nabla K_{\sigma^a}\big]\cdot\bar{\kappa}\cdot\big[N_{\sigma^a}\nabla G_{\sigma^a} - G_{\sigma^a}\nabla N_{\sigma^a}\big] \\
& + \big[K_{\sigma^a}\mathcal{L}^a_{\tilde{c}}(F) - F_{\sigma^a}\mathcal{L}^a_{\tilde{c}}(K)\big]\cdot\bar{D}\cdot\big[N_{\sigma^a}\mathcal{L}^a_{\tilde{c}}(G) - G_{\sigma^a}\mathcal{L}^a_{\tilde{c}}(N)\big].
\end{aligned}
$$

where a, of course, is not to be summed over and the pseudodifferential operator $\mathcal{L}^a_{\tilde{c}}$ has the following form:

$$
\mathcal{L}^a_{\tilde{c}}(F) := \nabla\big(F_{\tilde{c}} + \nabla\cdot(\rho^a\lambda_s\Gamma\boldsymbol{\zeta}F_{\sigma^a})/\rho\big)\,. \tag{3.152}
$$

Upon insertion of H^a as given by (3.116) and S from the set of Casimirs to be as in (3.117), the dynamics is given by

$$
\partial_t\xi^\alpha = \{\xi^\alpha, H^a\}^a + (\psi^\alpha, H^a; S^a, H^a)^a\,. \tag{3.153}
$$

Using $\mathcal{L}^a_{\tilde{c}}(H^a) = \nabla\mu^a_\Gamma$, $H^a_{\mathbf{m}} = \mathbf{v}$, $H^a_{\sigma_a} = T$, $S^a_{\sigma_a} = 1$ and $\mathcal{L}^a_{\tilde{c}}(S^a) = 0$, the following

diffuse-interface CHNS system for $a = 1$ is produced:

$$\begin{aligned}
\partial_t \mathbf{v} &= \{\mathbf{v}, H^1\}^1 + (\mathbf{v}, H^1; S^1, H^1)^1 \\
&= -\mathbf{v}\cdot\nabla\mathbf{v} - \frac{1}{\rho}\nabla\cdot\left[p\mathbf{I} + \lambda_f\rho\Gamma\boldsymbol{\zeta}\otimes\nabla c\right] + \frac{1}{\rho}\nabla\cdot(\bar{\bar{\Lambda}}:\nabla\mathbf{v})\,, && (3.154)\\
\partial_t \rho &= \{\rho, H^1\}^1 + (\rho, H^1; S^1, H^1)^1 \\
&= -\mathbf{v}\cdot\nabla\rho - \rho\,\nabla\cdot\mathbf{v}\,, && (3.155)\\
\partial_t \tilde{c} &= \{\tilde{c}, H^1\}^1 + (\tilde{c}, H^1; S^1, H^1)^1 \\
&= -\mathbf{v}\cdot\nabla\tilde{c} - \tilde{c}\,\nabla\cdot\mathbf{v} + \nabla\cdot(\bar{D}\cdot\nabla\mu^1_\Gamma)\,, && (3.156)\\
\partial_t \sigma^1_{\text{Total}} &= \{\sigma^1_{\text{Total}}, H^1\}^1 + (\sigma^1_{\text{Total}}, H^1; S^1, H^1)^1 \\
&= -\mathbf{v}\cdot\nabla\sigma^1_{\text{Total}} - \sigma^1_{\text{Total}}\,\nabla\cdot\mathbf{v} && (3.157)\\
&\quad + \nabla\cdot\left(\frac{\bar{\kappa}}{T}\cdot\nabla T\right) + \frac{1}{T^2}\nabla T\cdot\bar{\kappa}\cdot\nabla T && (3.158)\\
&\quad + \frac{1}{T}\nabla\mathbf{v}:\bar{\bar{\Lambda}}:\nabla\mathbf{v} + \frac{1}{T}\nabla\mu^1_\Gamma\cdot\bar{D}\cdot\nabla\mu^1_\Gamma\,. && (3.159)
\end{aligned}$$

Similarly, for $a = 0$ we obtain

$$\begin{aligned}
\partial_t \mathbf{v} &= \{\mathbf{v}, H^0\}^0 + (\mathbf{v}, H^0; S^0, H^0)^0 \\
&= -\mathbf{v}\cdot\nabla\mathbf{v} - \frac{1}{\rho}\nabla\cdot\left[\left(p - \lambda_f\Gamma^2/2\right)\mathbf{I} + \lambda_f\Gamma\boldsymbol{\zeta}\otimes\nabla c\right] + \frac{1}{\rho}\nabla\cdot(\bar{\bar{\Lambda}}:\nabla\mathbf{v})\,, && (3.160)\\
\partial_t \rho &= \{\rho, H^0\}^0 + (\rho, H^0; S^0, H^0)^0 \\
&= -\mathbf{v}\cdot\nabla\rho - \rho\,\nabla\cdot\mathbf{v}\,, && (3.161)\\
\partial_t \tilde{c} &= \{\tilde{c}, H^0\}^0 + (\tilde{c}, H^0; S^0, H^0)^0 \\
&= -\mathbf{v}\cdot\nabla\tilde{c} - \tilde{c}\,\nabla\cdot\mathbf{v} + \nabla\cdot(\bar{D}\cdot\nabla\mu^0_\Gamma)\,, && (3.162)\\
\partial_t \sigma^0_{\text{Total}} &= \{\sigma^0_{\text{Total}}, H^0\}^0 + (\sigma^0_{\text{Total}}, H^0; S^0, H^0)^0 \\
&= -\mathbf{v}\cdot\nabla\sigma^0_{\text{Total}} - \sigma^0_{\text{Total}}\,\nabla\cdot\mathbf{v} && (3.163)\\
&\quad + \nabla\cdot\left(\frac{\bar{\kappa}}{T}\cdot\nabla T\right) + \frac{1}{T^2}\nabla T\cdot\bar{\kappa}\cdot\nabla T + \frac{1}{T}\nabla\mathbf{v}:\bar{\bar{\Lambda}}:\nabla\mathbf{v} \\
&\quad + \frac{1}{T}\nabla\mu^0_\Gamma\cdot\bar{D}\cdot\nabla\mu^0_\Gamma\,. && (3.164)
\end{aligned}$$

Thus we have extracted from our general system with arbitrary a, two thermodynamically consistent CHNS systems. By construction both the $a = 1$ and $a = 0$ systems must conserve energy and both must produce entropy, which we find is

governed by the following:

$$\begin{aligned}\dot{S}^a &= (S^a, H^a; S^a, H^a)^a \\ &= \int_\Omega \frac{1}{T}\left[\nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v} + \frac{1}{T}\nabla T \cdot \bar{\kappa} \cdot \nabla T + \nabla \mu^a_\Gamma \cdot \bar{D} \cdot \nabla \mu^a_\Gamma\right] \geq 0\,. \end{aligned} \tag{3.165}$$

3.5 AN ALTERNATIVE OF CHNS'S MODELING

An alternative but equivalent Hamiltonian formulation of the above systems exists, in fact, one that has a standard entropy functional of the form of (3.83). Given that the bracket of (3.136) was obtained via a transformation of the bracket of (3.68), we can transform it back from one that has (3.117) as a Casimir to the original that has (3.57) as a Casimir. However, to generate equivalent equations of motion, we would have to transform the Hamiltonian of (3.116) into a more complicated form. Tracing back through our transformations, we would replace the coordinate σ^a in the Hamiltonian by $\sigma - \rho^a \lambda_s \Gamma^2/2$, which means the internal energy becomes

$$u \mapsto u(\rho, (\sigma - \rho^a \lambda_s \Gamma^2/2)/\rho, \tilde{c}/\rho)\,, \tag{3.166}$$

while otherwise the Hamiltonian remains the same. Just as with finite-dimensional Hamiltonian systems, one can change coordinates and arrive at equivalent systems with different Poisson brackets and Hamiltonians, and in the noncanonical case different expressions for the Casimir invariants. Often one has the options of a simple bracket and complicated Hamiltonian or vice verse. In the next section, we will proceed the UT-algorithm for the $a = 0$ case, with the options of a simple noncanonical Poisson bracket and usual entropy functional but complicated Hamiltonian functional.

• First step of UT-algorithm: We choose our dynamical variables as the following

$$\boldsymbol{\xi}(\mathbf{x}, t) = (\rho(\mathbf{x}, t), \mathbf{m}(\mathbf{x}, t), \tilde{c}(\mathbf{x}, t), \bar{\sigma}(\mathbf{x}, t)) \tag{3.167}$$

where again the mixture of two phases is assumed to be contained in a volume Ω, with coordinate $\mathbf{x}$, and to the densities $\rho, \mathbf{m}$, and $\bar{\sigma}$ used as in Sec. 3.1 we add $\tilde{c}$. Again we have singled out the entropy density $\bar{\sigma}$ as the last variable of $\boldsymbol{\xi}$, consistent with (2.62). (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 (2.63), we take the total entropy to be the integral of the last component

$$S = \int_\Omega \bar{\sigma}\,. \tag{3.168}$$

It was shown in Zaidni et al. [2024] that this simple entropy can be used instead of complicated entropy expressions used in Anderson et al. [2000, 1998], Anderson and McFadden [1996], Guo and Lin [2015], 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.

$$\bar{\sigma} = \sigma + \frac{\lambda_s}{2}\,\Gamma^2(\nabla c)\,. \tag{3.169}$$

Any Hamiltonian $H[\rho, \mathbf{m}, \tilde{c}, \bar{\sigma}]$ would be possible; however, as also shown in Zaidni et al. [2024], the price paid for a simplified entropy is the following complicated Hamiltonian:

$$H = \int_\Omega \frac{|\mathbf{m}|^2}{2\rho} + \rho\, u\big(\rho, \sigma/\rho, \tilde{c}/\rho\big) + \frac{\lambda_u}{2}\,\Gamma^2\big(\nabla(\tilde{c}/\rho)\big)\,, \tag{3.170}$$

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 (3.169),

$$H = \int_\Omega \frac{|\mathbf{m}|^2}{2\rho} + \rho\, u\big(\rho, \frac{\bar{\sigma}}{\rho} - \frac{\lambda_s}{2\rho}\,\Gamma^2(\nabla c), \tilde{c}/\rho\big) + \frac{\lambda_u}{2}\,\Gamma^2\big(\nabla(\tilde{c}/\rho)\big)\,, \tag{3.171}$$

From this extensive internal energy function, we obtain the intensive thermodynamical variables including the chemical potential as

$$p = \rho^2 \frac{\partial u}{\partial \rho}\,, \qquad T = \frac{\partial u}{\partial s}\,, \qquad \text{and} \qquad \mu = \frac{\partial u}{\partial c}\,. \tag{3.172}$$

where now $s = \bar{\sigma}/\rho$ and recall $c = \tilde{c}/\rho$.

• 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 Zaidni et al. [2024]. This bracket, which is a natural generalization of that given in Morrison and

Greene [1980], is given by

$$\begin{aligned}\{F,G\} = -\int_\Omega \mathbf{m}\cdot[F_{\mathbf{m}}\cdot\nabla G_{\mathbf{m}} - G_{\mathbf{m}}\cdot\nabla F_{\mathbf{m}}] \\ + \rho\,[F_{\mathbf{m}}\cdot\nabla G_\rho - G_{\mathbf{m}}\cdot\nabla F_\rho] \\ + \bar\sigma\,[F_{\mathbf{m}}\cdot\nabla G_{\bar\sigma} - G_{\mathbf{m}}\cdot\nabla F_{\bar\sigma}] \\ + \tilde c\,[F_{\mathbf{m}}\cdot\nabla G_{\tilde c} - G_{\mathbf{m}}\cdot\nabla F_{\tilde c}]\,. \end{aligned} \tag{3.173}$$

It is simple to verify that the S of (3.168) is a Casimir invariant of this bracket.

• Fourth step of UT-algorithm: To construct the metriplectic 4-bracket, we proceed as in Sec. 3.1 with the forms of M and Σ given by (3.6) and (3.7), albeit with $\bar\sigma$ replacing σ in (3.6). 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 (2.61):

$$\begin{aligned}\mathbf{J}_\rho &= -L^{\rho\rho}\cdot\mathcal{L}_*^\rho(H_\rho) - L^{\rho\mathbf{m}}\colon\mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\rho\sigma}\cdot\mathcal{L}_*^{\bar\sigma}(H_{\bar\sigma}) - L^{\rho\tilde c}\cdot\mathcal{L}_*^{\tilde c}(H_{\tilde c})\,,\\ \bar J_{\mathbf{m}} &= -L^{\mathbf{m}\rho}\otimes\mathcal{L}_*^\rho(H_\rho) - L^{\mathbf{mm}}:\mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\mathbf{m}\sigma}\otimes\mathcal{L}_*^{\bar\sigma}(H_{\bar\sigma}) - L^{\mathbf{m}\tilde c}\otimes\mathcal{L}_*^{\tilde c}(H_{\tilde c})\,,\\ \mathbf{J}_c &= -L^{\tilde c\rho}\cdot\mathcal{L}_*^\rho(H_\rho) - L^{\tilde c\mathbf{m}}\colon\mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\tilde c\bar\sigma}\cdot\mathcal{L}_*^{\bar\sigma}(H_{\bar\sigma}) - L^{\tilde c\tilde c}\cdot\mathcal{L}_*^{\tilde c}(H_{\tilde c})\,,\\ \mathbf{J}_s &= -L^{\bar\sigma\rho}\cdot\mathcal{L}_*^\rho(H_\rho) - L^{\bar\sigma\mathbf{m}}\colon\mathcal{L}_*^{\mathbf{m}}(H_{\mathbf{m}}) - L^{\bar\sigma\bar\sigma}\cdot\mathcal{L}_*^{\bar\sigma}(H_{\bar\sigma}) - L^{\bar\sigma\tilde c}\cdot\mathcal{L}_*^{\tilde c}(H_{\tilde c})\,.\end{aligned} \tag{3.174}$$

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 $\mathcal{L}_*^\alpha$.

Now we specialize and show that the general expressions for the fluxes of (3.174) 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 (3.170), then we obtain the CHNS system of Anderson et al. [Anderson et al., 2000, 1998, Anderson and McFadden, 1996] (see also Zaidni et al. [2024]). Using

$$\begin{aligned}H_\rho = -\frac{|\mathbf{m}|^2}{2\rho^2} + u + \rho u_\rho - \left(\frac{\sigma}{\rho} - \frac{\lambda_s}{2\rho}\Gamma^2\right)u_s - \frac{\tilde c}{\rho}u_c \\ + \frac{\tilde c}{\rho^2}\nabla\cdot(u_s\lambda_s\Gamma\boldsymbol{\zeta}) + \frac{\tilde c}{\rho^2}\nabla\cdot(\Gamma\boldsymbol{\zeta}\lambda_u)\end{aligned} \tag{3.175}$$

$$H_{\tilde c} = u_c + \frac{\lambda_s}{\rho}\nabla\cdot(u_s\Gamma\boldsymbol{\zeta}) - \frac{1}{\rho}\nabla\cdot(\lambda_s\Gamma\boldsymbol{\zeta}) =: \mu_\Gamma\,, \tag{3.176}$$

$$H_{\mathbf{m}} = \mathbf{v}, \qquad H_{\bar\sigma} = u_s = T\,., \tag{3.177}$$

where, from (3.101), 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

$$L^{\mathbf{mm}} = \bar{\bar{\Lambda}}\,, \quad L^{\bar{\sigma}\bar{\sigma}} = \frac{\bar{\kappa}}{T}\,, \quad \text{and} \quad L^{\tilde{c}\tilde{c}} = \bar{D}\,. \tag{3.178}$$

Equations (3.174) for the fluxes reduce to the following form:

$$\mathbf{J}_\rho = 0\,, \tag{3.179}$$

$$\bar{J}_{\mathbf{m}} = -\bar{\bar{\Lambda}} : \nabla\mathbf{v}\,, \tag{3.180}$$

$$\mathbf{J}_c = -\bar{D}\cdot\nabla\mu_\Gamma\,, \tag{3.181}$$

$$\mathbf{J}_s = -\frac{\bar{\kappa}}{T}\cdot\nabla T\,, \tag{3.182}$$

where $\mu_\Gamma := \mu - \frac{1}{\rho}\nabla\cdot(\lambda_f\Gamma\boldsymbol{\zeta})$. Equations are the known fluxes for the CHNS system of Anderson et al. [2000, 1998], Anderson and McFadden [1996].

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

$$M(dF, dG) = F_{\bar{\sigma}}G_{\bar{\sigma}}\,, \tag{3.183}$$

$$\Sigma(dF, dG) = \nabla F_{\mathbf{m}} : \bar{\bar{\Lambda}} : \nabla G_{\mathbf{m}} + \nabla F_{\bar{\sigma}}\cdot\frac{\bar{\kappa}}{T^2}\cdot\nabla G_{\bar{\sigma}} + \nabla(F_{\tilde{c}})\cdot\frac{\bar{D}}{T}\cdot\nabla(G_{\tilde{c}})\,, \tag{3.184}$$

is given by

$$\begin{aligned}(F, K; G, N) = \int_\Omega \frac{1}{T}\Big[\,&[K_{\bar{\sigma}}\nabla F_{\mathbf{m}} - F_{\bar{\sigma}}\nabla K_{\mathbf{m}}]:\bar{\bar{\Lambda}}:[N_{\bar{\sigma}}\nabla G_{\mathbf{m}} - G_{\bar{\sigma}}\nabla N_{\mathbf{m}}] \\ &+ \frac{1}{T}\big[K_{\bar{\sigma}}\nabla F_{\bar{\sigma}} - F_{\bar{\sigma}}\nabla K_{\bar{\sigma}}\big]\cdot\bar{\kappa}\cdot\big[N_{\bar{\sigma}}\nabla G_{\bar{\sigma}} - G_{\bar{\sigma}}\nabla N_{\bar{\sigma}}\big] \\ &+ \big[K_{\bar{\sigma}}\nabla F_{\tilde{c}} - F_{\bar{\sigma}}\nabla K_{\tilde{c}}\big]\cdot\bar{D}\cdot\big[N_{\bar{\sigma}}\nabla G_{\tilde{c}} - G_{\bar{\sigma}}\nabla N_{\tilde{c}}\big].\end{aligned} \tag{3.185}$$

Upon insertion of H as given by (3.170) and S given by (3.168), using (3.175),

(3.176), and (3.177) with $S_{\bar{\sigma}} = 1$, the following CHNS system is produced

$$\begin{aligned}
\partial_t \rho &= \{\rho, H\} + (\rho, H; S, H) \\
&= -\mathbf{v} \cdot \nabla \rho - \rho \nabla \cdot \mathbf{v} \,, \qquad (3.186) \\
\partial_t \mathbf{v} &= \{\mathbf{v}, H\} + (\mathbf{v}, H; S, H) \\
&= -\mathbf{v} \cdot \nabla \mathbf{v} - \frac{1}{\rho} \nabla \cdot \Big[\big(p - \lambda_f \Gamma^2/2\big) \bar{I} + \lambda_f \Gamma \boldsymbol{\zeta} \otimes \nabla c \Big] + \frac{1}{\rho} \nabla \cdot (\bar{\bar{\Lambda}} : \nabla \mathbf{v}) \,, \qquad (3.187) \\
\partial_t \tilde{c} &= \{\tilde{c}, H\} + (\tilde{c}, H; S, H) \\
&= -\mathbf{v} \cdot \nabla \tilde{c} - \tilde{c} \nabla \cdot \mathbf{v} + \nabla \cdot (\bar{D} \cdot \nabla \mu_\Gamma^0) \,, \qquad (3.188) \\
\partial_t \bar{\sigma} &= \{\bar{\sigma}, H\} + (\bar{\sigma}, H; S, H) \\
&= -\mathbf{v} \cdot \nabla \bar{\sigma} - \bar{\sigma} \nabla \cdot \mathbf{v} + \nabla \cdot \Big(\frac{\bar{\kappa}}{T} \cdot \nabla T \Big) + \frac{1}{T^2} \nabla T \cdot \bar{\kappa} \cdot \nabla T \qquad (3.189) \\
&\qquad + \frac{1}{T} \nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v} + \frac{1}{T} \nabla \mu_\Gamma \cdot \bar{D} \cdot \nabla \mu_\Gamma \,.
\end{aligned}$$

where $\bar{I}$ is the identity and recall $\boldsymbol{\xi}$ is defined in (3.122),

$$\mu_\Gamma \coloneqq u_c + \frac{\lambda_s}{\rho} \nabla \cdot (u_s \Gamma \boldsymbol{\zeta}) - \frac{1}{\rho} \nabla \cdot (\lambda_s \Gamma \boldsymbol{\zeta}) \,, \qquad (3.190)$$

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:

$$\begin{aligned}
\dot{S} &= (S, H; S, H) \\
&= \int_\Omega \frac{1}{T} \Big[\nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v} + \frac{1}{T} \nabla T \cdot \bar{\kappa} \cdot \nabla T + \nabla \mu_\Gamma \cdot \bar{D} \cdot \nabla \mu_\Gamma \Big] \geq 0 \,, \qquad (3.191)
\end{aligned}$$

whence it is seen to be produced.

In Sec. 3.4.1 the entropy of (3.117) was simplified to the standard form of (3.168) by a coordinate change. This resulted in the more complicated internal energy function of (3.170), as compared with (3.116), 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.

A cornerstone of Hamiltonian dynamics is its geometric invariance under coordinate changes. Because the minimal metriplectic properties are algebraic and geometric, they too are invariant under coordinate changes. Thus, we can write our CHNS class of dissipative systems with a standard entropy functional of the form of (3.83), but with a more complicated Hamiltonian using (3.166).

3.6 DISCUSSION AND CONCLUSION

From the examples presented in this chapter, it is clear that the 4-bracket formalism can be applied to obtain a wide variety of dynamical systems in various fields. In fact it was recently applied to obtain generalized collision operators in kinetic theory [Sato and Morrison, 2024] and a thermodynamically consistent model for radiation hydrodynamics [Tran et al., 2024]. Although incompressible flows don't have the usual thermodynamics associated with compression and pressure, they can be included in the metriplectic formalism by using the techniques of Chandre et al. [2013].

The main contribution in this chapter is the unified thermodynamical algorithm (UTA) that uses the metriplectic 4-bracket of previous work [Morrison and Updike, 2024, Zaidni et al., 2024, Sato and Morrison, 2024] 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 (2.61). In Sec. 3 we present examples that generalize previous results. In particular, we showed that the Brenner-Navier-Stokes-Fourier system and its generalization of Reddy et al. [2019] 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 (2.67). One clear distinction can be made: that between Hamiltonian vs. nonHamiltonian, 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 [Morrison, 1984a], 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 Öttinger [2005]. A resolution of this dichotomy is achieved with the UTA, where temperature may appear according to (2.67) and (2.79) 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 [Mills, 2006] 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 [Sato and Morrison, 2024] 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 UTA 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 (2.12) or (2.61). 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 (2.12) or (2.61) by using rectification arguments similar to those described in [Morrison and Updike, 2024]. 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.

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 that 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.

In the next chapter, we will see that the metriplectic 4-bracket formalism also provides an avenue for designing structure preserving numerical algorithms [see e.g. Morrison, 2017]. Any discretization that preserves the symmetries of the 4-bracket,

which is not a difficult task, will be thermodynamically consistent on the semi-discrete level, i.e. produce a set of ordinary differential equations that conserve energy and produce entropy. For simplicity, we have chosen to make a discretization of Navier-Stokes-Fourier equations in one dimension using their metriplectic formalism.

CHAPTER

NUMERICAL SCHEME USING METRIPLECTIC FORMALISM 4

4.1 INTRODUCTION

The Navier-Stokes-Fourier system is known to satisfy the first and second laws of thermodynamics. Therefore, it is desirable that a numerical scheme for this system should likewise be consistent with the laws of thermodynamics. In this chapter we derive such a scheme in one spatial dimension by preserving the symmetries of the Poisson bracket and the metriplectic 4-bracket formulation of the model in its spatial discretization.

The metriplectic 2-bracket has previously been used in the discretization of collisional kinetic plasmas [Kraus and Hirvijoki, 2017, Jeyakumar et al., 2024], and the calculation of MHD equilibria [Bressan et al., 2018]. The formalism has also been employed in reduced order modeling [Gruber et al., 2023]. Previous thermodynamically consistent discretizations of thermal-fluid models have been derived based on the Lagrange d'Alembert principle, a dissipative extension of Lagrangian mechanics [Gawlik and Gay-Balmaz, 2024]. There is also prior work considering thermodynamic consistency in the context of sub-grid parameterizations in atmospheric modeling [Gassmann and Herzog, 2015]. This paper is the first to use a metriplectic 4-bracket in the design of a numerical method.

It is worth mentioning that the natural variables for fluid models using the metriplectic formulation use entropy rather than internal energy as a prognostic variable. This makes our formulation incompatible with many tools in common

practice for numerical methods for hyperbolic conservation laws. Standard methods use conservation form to great effect in deriving finite difference [Richtmyer and Morton, 1967, Toro, 2013], finite volume [Toro, 2013, LeVeque, 2002], and discontinuous Galerkin methods [Cockburn and Shu, 2001, Hesthaven and Warburton, 2008], with well-developed stabilization techniques for shocks inextricably connected to the use of conservation form. However, there is precedent in the literature for using a skew-symmetric split form—a weak formulation that incorporates both the advective and conservative forms of the transport operator—rather than solely using conservative form to simulate fluid models [Morinishi et al., 1998, Gassner, 2013, Gassner and Winters, 2014, Palha et al., 2017]. Similar to this work, the motivation for employing these split forms is to construct invariant-preserving schemes. Moreover, prior studies have explored the use of entropy, rather than total energy, as a prognostic variable in compressible flow simulations (see Shakib et al. [1991] and references therein). While this work builds on prior research, the approach proposed herein does not aim to compete with the state-of-the-art methods based on conservation form without substantial further research addressing the need for stabilization and shock-capturing techniques tailored to this formalism.

4.2 A THERMAL-FLUID MODEL AND ITS METRIPLECTIC STRUCTURE

A thermodynamically-consistent model of compressible flow, frequently called the Navier-Stokes-Fourier system, was shown to possess metriplectic 4-bracket structure in Sec.3.1. In a single spatial dimension, the equations of motion are given by

$$\begin{aligned}
&\partial_t \rho + \partial_x(\rho u) = 0\,, \\
&\partial_t(\rho u) + \partial_x(\rho u^2) + \partial_x p = \partial_x(\mu \partial_x u)\,, \\
&\partial_t(\rho s) + \partial_x(\rho s u) = \frac{\mu}{T}(\partial_x u)^2 + \partial_x\left(\frac{\kappa}{T}\partial_x T\right) + \frac{\kappa}{T^2}(\partial_x T)^2\,,
\end{aligned} \tag{4.1}$$

where μ and κ are the viscosity and thermal-conductivity coefficients, respectively, and there exists an internal energy $U = U(\rho, s)$ such that the pressure and temperature are prescribed by $p = \rho^2 \partial_\rho U$ and $T = \partial_s U$. It may be shown that this model possesses a metriplectic structure.

It is convenient to use density coordinates: $(\rho, m, \sigma) = (\rho, \rho u, \rho s)$ when writing the metriplectic structure of the Navier-Stokes-Fourier system. The Hamiltonian is

given by

$$H[\rho, m, \sigma] = \int_\Omega \left(\frac{1}{2}\frac{m^2}{\rho} + \rho U\left(\rho, \frac{\sigma}{\rho}\right)\right) \mathsf{d}x\,, \tag{4.2}$$

and, using the functional derivative shorthand $\delta F/\delta u = F_u$, the Poisson bracket is given by

$$\begin{aligned}\{F, G\} = -\int_\Omega \Big[& m\left(F_m \partial_x G_m - G_m \partial_x F_m\right) + \rho\left(F_m \partial_x G_\rho - G_m \partial_x F_\rho\right) \\ & + \sigma\left(F_m \partial_x G_\sigma - G_m \partial_x F_\sigma\right)\Big] \mathsf{d}x\,. \end{aligned} \tag{4.3}$$

Assuming homogeneous or periodic boundary conditions, the evolution law $\dot{F} = \{F, H\}$ for arbitrary $F = F[\rho, m, \sigma]$ recovers the conservative part of the dynamics given by the right-hand side of equation (4.1). This Poisson bracket possesses a Casimir invariant of the form $S[\rho, m, \sigma] = \int_\Omega \sigma \mathsf{d}x$. This is the total entropy, and is used as the generator for the dissipative dynamics.

The metriplectic structure is prescribed by a 4-bracket constructed using the Kulkarni-Nomizu product (see e.g. Morrison and Updike [2023], Zaidni et al. [2024], Zaidni and Morrison [2024]) from the following symmetric operators:

$$M(F, G) = F_\sigma G_\sigma\,, \quad \text{and} \quad \Sigma(F, G) = (\partial_x F_m)\frac{\mu}{T}(\partial_x G_m) + (\partial_x F_\sigma)\frac{\kappa}{T^2}(\partial_x G_\sigma)\,. \tag{4.4}$$

The Kulkarni-Nomizu product is given by

$$\begin{aligned}(\Sigma \wedge M)(F, K, G, N) = {} & \Sigma(F, G)M(K, N) - \Sigma(F, N)M(G, K) \\ & + M(F, G)\Sigma(K, N) - M(F, N)\Sigma(G, K)\,, \end{aligned} \tag{4.5}$$

from which one then defines the 4-bracket:

$$\begin{aligned}(F, K; G, N) &= \int_\Omega (\Sigma \wedge M)(F, K, G, N) \mathsf{d}x \\ &= \int_\Omega \frac{1}{T}\Big[\mu\left(K_\sigma \partial_x F_m - F_\sigma \partial_x K_m\right)\left(N_\sigma \partial_x G_m - G_\sigma \partial_x N_m\right) \\ &\qquad + \frac{\kappa}{T}\left(K_\sigma \partial_x F_\sigma - F_\sigma \partial_x K_\sigma\right)\left(N_\sigma \partial_x G_\sigma - G_\sigma \partial_x N_\sigma\right)\Big] \mathsf{d}x\,. \end{aligned} \tag{4.6}$$

The rationale for choosing the operators M and Σ as given in (4.4) comes from a

closer examination of the implied dissipative evolution:

$$(F,S)_H = \int_\Omega (\Sigma \wedge M)(F,K,G,N)\mathsf{d}x = \int_\Omega \left(-\Sigma(F,H)M(S,H) + M(F,S)\Sigma(H,H)\right)\mathsf{d}x$$
$$= \int_\Omega \Big(- \Big[(\partial_x F_m)\mu\partial_x u + (\partial_x F_\sigma)\frac{\kappa}{T}(\partial_x T)\Big] + F_\sigma\left[\frac{\mu}{T}(\partial_x u)^2 + \frac{\kappa}{T^2}(\partial_x T)^2\right]\Big)\,\mathsf{d}x\,. \tag{4.7}$$

By letting $M = F_\sigma G_\sigma$, we find that $\Sigma(H,H)$ is the entropy production rate while $\Sigma(F,H)$ gives rise to the reciprocal couplings which ensure energy conservation. This rationale for finding the metriplectic 4-bracket is generally applicable for many compressible flow models, see [Morrison and Updike, 2023, Zaidni and Morrison, 2024], and directly connects with standard arguments from non-equilibrium thermodynamics [de Groot and Mazur, 1962], e.g. the force and flux pairs from Onsager reciprocity.

The metriplectic 2-bracket is then defined to be $(F,G)_H \coloneqq (F,H;G,H)$. The evolution law $\dot{F} = \{F,H\} + (F,S)_H$ for arbitrary $F = F[\rho,m,\sigma]$ recovers the full Navier-Stokes-Fourier system. To be explicit, one finds that

$$\{F,H\} = -\int_\Omega \Big[m\left(F_m\partial_x u - u\partial_x F_m\right) + \rho\left(F_m\partial_x\eta - m\partial_x F_\rho\right) + \sigma\left(F_m\partial_x T - u\partial_x F_\sigma\right)\Big]\mathsf{d}x\,, \tag{4.8}$$

where we used the fact that $H_m = m/\rho = u$, $H_\sigma = \partial_s U = T$, and

$$H_\rho \coloneqq \eta = \frac{m^2}{2\rho^2} + U + \rho U_\rho\left(\rho,\frac{\sigma}{\rho}\right) - \frac{\rho}{\sigma}U_s\left(\rho,\frac{\sigma}{\rho}\right)\,, \tag{4.9}$$

is related to the enthalpy. Combining this with the dissipative vector field implied by equation (4.7), we obtain the weak evolution equations:

$$\begin{aligned}\dot{F} &= \{F,H\} + (F,S)_H \\ &= -\int_\Omega \Big[m\left(F_m\partial_x u - u\partial_x F_m\right) + \rho\left(F_m\partial_x\eta - m\partial_x F_\rho\right) + \sigma\left(F_m\partial_x T - u\partial_x F_\sigma\right)\Big]\mathsf{d}x \\ &+ \int_\Omega \Big(- \Big[(\partial_x F_m)\mu\partial_x u + (\partial_x F_\sigma)\frac{\kappa}{T}(\partial_x T)\Big] + F_\sigma\left[\frac{\mu}{T}(\partial_x u)^2 + \frac{\kappa}{T^2}(\partial_x T)^2\right]\Big)\,\mathsf{d}x\,.\end{aligned} \tag{4.10}$$

Integration by parts and some algebraic manipulation recovers the strong evolution equations given in equation (4.1). However, it is this weak form in equation (4.10) implied by the Hamiltonian and metriplectic structure, and not the evolution equations themselves in equation (4.1), from which a thermodynamically-consistent finite element method will be derived.

It is convenient to non-dimensionalize the equations of motion. The viscosity and conductivity coefficients are assumed to be constant. Define the following dimensionless quantities:

$$\tilde{x} = \frac{x}{L}\,, \quad \tilde{u} = \frac{u}{V}\,, \quad \tilde{\rho} = \frac{\rho}{\rho_0}\,, \quad \tilde{\sigma} = \frac{\sigma}{\rho_0 R}\,, \quad \tilde{t} = \frac{Lt}{V}\,, \quad \tilde{p} = \frac{p}{\rho_0 V^2}\,, \quad \text{and} \quad \tilde{T} = \frac{RT}{\rho_0 V^2}\,, \tag{4.11}$$

where tildes indicate dimensionless quantities; L, V, and ρ_0 are taken to be the characteristic length, velocity, and density, respectively; and R is the ideal gas constant. Dropping the tildes for notational ease, the equations of motion become

$$\begin{aligned}
&\partial_t \rho + \partial_x(\rho u) = 0\,,\\
&\partial_t(\rho u) + \partial_x(\rho u^2) + \partial_x p = \frac{1}{\mathrm{Re}}\partial_x^2 u\,,\\
&\partial_t(\rho s) + \partial_x(\rho s u) = \frac{1}{\mathrm{Re}}\frac{(\partial_x u)^2}{T} + \frac{1}{\mathrm{Re}\,\mathrm{Pr}}\frac{\gamma}{\gamma-1}\left(\partial_x\left(\frac{1}{T}\partial_x T\right) + \frac{(\partial_x T)^2}{T^2}\right)\,,
\end{aligned} \tag{4.12}$$

where $\mathrm{Re} = (\rho_0 V L)/\mu$, $\mathrm{Pr} = \kappa/(\mu c_P)$, and $\gamma = c_p/c_v$ are the Reynolds number, Prandtl number, and heat capacity ratio respectively. Recall that $R/c_v = \gamma - 1$.

For the purposes of this paper, it is sufficient to consider the ideal gas equation of state. In dimensionless units, the internal energy is written $U(\rho, s) = \rho^{\gamma-1}e^{(\gamma-1)s}$ so that $p = \rho^2\partial_1 U = (\gamma-1)\rho^\gamma e^{(\gamma-1)\sigma/\rho}$, and $T = \partial_2 U = (\gamma-1)\rho^{\gamma-1}e^{(\gamma-1)\sigma/\rho}$, where ∂_i indicates differentiation with respect to the i^{th} argument. In these units $p = \rho T$ as required.

4.3 A THERMODYNAMICALLY CONSISTENT DISCRETIZATION

In this work, we consider simulations on a periodic domain: $\Omega = [0, L]/\!\sim$, where $L > 0$ and the equivalence relation identifies the endpoints. Let $V_h \subset H^1(\Omega)$ be the degree-p continuous Galerkin finite element space defined over a uniform grid, $\mathcal{T}_h$, on Ω: i.e.

$$V_h = \{v_h \in H^1(\Omega) : v_h|_K \in \mathbb{P}^p(K)\,, \forall K \in \mathcal{T}_h\}\,, \tag{4.13}$$

where $\mathbb{P}^p(K)$ is the space of degree-p polynomials on $K \subset \Omega$. The discretization is accomplished using the method of lines by positing that all dynamical fields have spatial dependence modeled in this Galerkin subspace. However, rather than discretizing the equations of motion themselves, we discretize the weak forms implied

by the metriplectic formulation.

Let $(\rho_h, m_h, \sigma_h) \in V_h \times V_h \times V_h$. The discretized Hamiltonian and entropy are given by

$$H^h[\rho_h, m_h, \sigma_h] = \int_\Omega \left[\frac{1}{2}\frac{m_h^2}{\rho_h} + \rho_h U\left(\rho_h, \frac{\sigma_h}{\rho_h}\right)\right] \mathsf{d}x\,, \quad S^h[\sigma_h] = \int_\Omega \sigma_h \mathsf{d}x\,, \tag{4.14}$$

the antisymmetric bracket is given by

$$\begin{aligned}\{F^h, G^h\}_h(\rho_h, m_h, \sigma_h) = -\int_\Omega \Big[& m_h \left(F^h_{m_h}\partial_x G^h_{m_h} - G^h_{m_h}\partial_x F^h_{m_h}\right) \\ & + \rho_h \left(F^h_{m_h}\partial_x G^h_{\rho_h} - G^h_{m_h}\partial_x F^h_{\rho_h}\right) + \sigma_h \left(F^h_{m_h}\partial_x G^h_{\sigma_h} - G^h_{m_h}\partial_x F^h_{\sigma_h}\right)\Big] \mathsf{d}x\,,\end{aligned} \tag{4.15}$$

and the metriplectic 4-bracket is given by

$$\begin{aligned}(F^h, K^h; G^h, N^h)_h = \frac{1}{\mathrm{Re}}\int_\Omega \frac{1}{T_h}\Big[& \left(K^h_{\sigma_h}\partial_x F^h_{m_h} - F^h_{\sigma_h}\partial_x K^h_{m_h}\right)\left(N^h_{\sigma_h}\partial_x G^h_{m_h} - G^h_{\sigma_h}\partial_x N^h_{m_h}\right) \\ & + \frac{1}{\mathrm{Pr}}\frac{\gamma}{\gamma-1}\frac{1}{T_h}\left(K^h_{\sigma_h}\partial_x F^h_{\sigma_h} - F^h_{\sigma_h}\partial_x K^h_{\sigma_h}\right)\left(N^h_{\sigma_h}\partial_x G^h_{\sigma_h} - G^h_{\sigma_h}\partial_x N^h_{\sigma_h}\right)\Big] \mathsf{d}x\,,\end{aligned} \tag{4.16}$$

where $F^h = F|_{V_h}$, and similarly for the other functionals. We call the bracket in equation (4.15) an antisymmetric bracket, and not a Poisson bracket, because it is fails to satisfy the Jacobi identity: i.e. the identity

$$\{F, \{G, H\}\} + \{H, \{F, G\}\} + \{G, \{H, F\}\} = 0 \quad \forall F, G, H\,. \tag{4.17}$$

This is an essential algebraic property of Poisson brackets. However, no grid-based discretization of the kinds of Poisson brackets found in fluid models (or indeed those of most Hamiltonian partial differential equations) which preserves the Jacobi identity is known. This deficiency motivates the use of the terminology “almost Poisson" sometimes found in the literature [Cotter, 2023] to describe discretizations of Poisson brackets which fail to satisfy the Jacobi identity. These discretizations nonetheless preserve antisymmetry and the Casimir invariants giving rise to mass and total entropy conservation, which is sufficient for the purposes of this work.

The functional derivatives of the Hamiltonian are as follows:

$$H^h_{\rho_h} = Q_{V_h}\bigg(-\frac{m_h^2}{2\rho_h^2} + U\left(\rho_h, \frac{\sigma_h}{\rho_h}\right) + \rho_h \partial_1 U\left(\rho_h, \frac{\sigma_h}{\rho_h}\right) - \frac{\rho_h}{\sigma_h}\partial_2 U\left(\rho_h, \frac{\sigma_h}{\rho_h}\right)\bigg),$$
$$H^h_{m_h} = Q_{V_h}\left(\frac{m_h}{\rho_h}\right), \quad \text{and} \quad H^h_{\sigma_h} = Q_{V_h}\left(\partial_2 U\left(\rho_h, \frac{\sigma_h}{\rho_h}\right)\right), \tag{4.18}$$

where Q_{V_h} is the L^2 projection onto V_h. These derivatives must be projected because the functional derivatives are taken with respect to constrained variations in the space V_h. Similarly, one finds $S^h_{\rho_h} = S^h_{m_h} = 0$, and $S^h_{\sigma_h} = 1$, since V_h interpolates constant functions exactly. For convenience, and to match notation used subsequently, we write $\delta \boldsymbol{s}_h = (0, 0, 1)$ to denote the vector of derivatives of the entropy with respect to the three dynamical fields, (ρ_h, m_h, σ_h).

The evolution is then given by $\dot{F}^h = \{F^h, H^h\}_h + (F^h, H^h; S^h, H^h)_h$. One immediately finds that the semi-discrete model is thermodynamically consistent, $\dot{H}^h = 0$ and $\dot{S}^h \geq 0$, as the discretized brackets possess the same symmetries and degeneracies as the continuous brackets. If we consider an observable of the form $F^h = (\phi_m, m_h)_{L^2} + (\phi_\rho, \rho_h)_{L^2} + (\phi_\sigma, \sigma_h)_{L^2}$, then we obtain the following variational problem: find $(\boldsymbol{u}_h, \delta \boldsymbol{h}_h) \coloneqq ((\rho_h, m_h, \sigma_h), (\eta_h, u_h, T_h)) \in V_h^3 \times V_h^3$, where $V_h^3 = V_h \times V_h \times V_h$, such that

$$(\boldsymbol{v}_h, \partial_t \boldsymbol{u}_h)_{L^2} - \{\boldsymbol{v}_h, \delta \boldsymbol{h}_h\}(\boldsymbol{u}_h) - (\boldsymbol{v}_h, \delta \boldsymbol{s}_h)_H(\delta \boldsymbol{h}_h) + (\delta \boldsymbol{h}_h - DH(\boldsymbol{u}_h), \boldsymbol{w}_h)_{L^2} = 0 \tag{4.19}$$

$\forall (\boldsymbol{v}_h, \boldsymbol{w}_h) \coloneqq ((\phi_\rho, \phi_m, \phi_\sigma), (\phi_{\eta_h}, \phi_{u_h}, \phi_{T_h})) \in V_h^3 \times V_h^3$, where

$$(\boldsymbol{v}_h, \partial_t \boldsymbol{u}_h)_{L^2} = (\partial_t \rho_h, \phi_\rho)_{L^2} + (\partial_t m_h, \phi_m)_{L^2} + (\partial_t \sigma_h, \phi_\sigma)_{L^2}, \tag{4.20}$$

the discrete Poisson bracket is defined to be

$$\{\boldsymbol{v}_h, \delta \boldsymbol{h}_h\}(\boldsymbol{u}_h) = \{F^h, H^h\}_h(\boldsymbol{u}_h) = -(m_h \partial_x u_h, \phi_m)_{L^2} + (m_h u_h, \partial_x \phi_m)_{L^2}$$
$$- (\rho_h \partial_x \eta_h, \phi_m)_{L^2} + (\rho_h u_h, \partial_x \phi_\rho)_{L^2} - (\sigma_h \partial_x T_h, \phi_m)_{L^2} + (\sigma_h u_h, \partial_x \phi_\sigma)_{L^2}, \tag{4.21}$$

the discrete metriplectic bracket yields

$$(\boldsymbol{v}_h, \delta \boldsymbol{s}_h)_H(\delta \boldsymbol{h}_h) = (F^h, H^h; S^h, H^h)_h = -\frac{1}{\mathrm{Re}}\bigg[(\partial_x u_h, \partial_x \phi_m)_{L^2} - \left(\frac{(\partial_x u_h)^2}{T_h}, \phi_\sigma\right)_{L^2}$$
$$+ \frac{1}{\mathrm{Pr}}\frac{\gamma}{\gamma - 1}\bigg[\left(\frac{\partial_x T_h}{T_h}, \partial_x \phi_\sigma\right)_{L^2} - \left(\frac{(\partial_x T_h)^2}{T_h^2}, \phi_\sigma\right)_{L^2}\bigg]\bigg], \tag{4.22}$$

and the L^2 projections of the derivatives of the Hamiltonian are imposed via

$$(\delta \boldsymbol{h}_h - DH(\boldsymbol{u}_h), \boldsymbol{w}_h)_{L^2} = \left(\eta_h - \frac{\delta H^h}{\delta \rho_h}, \phi_{\eta_h}\right)_{L^2} + \left(u_h - \frac{\delta H^h}{\delta m_h}, \phi_{u_h}\right)_{L^2} + \left(T_h - \frac{\delta H^h}{\delta \sigma_h}, \phi_{T_h}\right)_{L^2} . \tag{4.23}$$

This notation attempts to stress three essential features of the spatial discretization.

- The derivatives of the generating functions are computed as via projections and must be thought of as distinct from the evolving state vector, $\boldsymbol{u}_h = (\rho_h, m_h, \sigma_h)$. Hence, we keep track of the derivatives of the Hamiltonian, $\delta \boldsymbol{h}_h = (\eta_h, m_h, T_h)$, as additional degrees of freedom (note, $\delta \boldsymbol{s}_h = (0, 0, 1)$ takes a simple form in momentum coordinates).

- The bilinear two-brackets generating the conservative and dissipative dynamics,

  $$\{\boldsymbol{v}_h, \delta \boldsymbol{h}_h\}(\boldsymbol{u}_h) \quad \text{and} \quad (\boldsymbol{v}_h, \delta \boldsymbol{s}_h)_H(\delta \boldsymbol{h}_h) , \tag{4.24}$$

  respectively, take the derivatives of the generating functions, $\delta \boldsymbol{h}_h$ and $\delta \boldsymbol{s}_h$, as one argument, and arbitrary the test function, $\boldsymbol{v}_h$ as the other.

- These brackets also have nonlinear field dependence. The discrete antisymmetric bracket depends directly on the state-vector, $\boldsymbol{u}_h$, while the discrete symmetric bracket depends on the derivative of the Hamiltonian, $\delta \boldsymbol{h}_h$. The nonlinear dependence of the dissipative bracket on $\delta \boldsymbol{h}_h$, rather than $\boldsymbol{u}_h$, is dictated by the 4-bracket formalism and essential for energy conservation.

By including the L^2 projection of the derivatives of the Hamiltonian as additional fields to solve for in the variational problem, we formulate the semi-discrete problem as a differential algebraic equation. The derivatives of the Hamiltonian with respect to momentum and entropy density have the physical interpretation of being the velocity and temperature, respectively. The derivative of the Hamiltonian with respect to density is related to the enthalpy, and one may readily recover the gradient of the pressure through a Bernoulli-like equation:

$$\left(\partial_x p_h + \frac{1}{2}\partial_x(u_h^2) - \rho_h \partial_x \eta_h + \sigma_h \partial_x T_h, \phi\right)_{L^2} = 0 , \quad \forall \phi \in V_h . \tag{4.25}$$

To be perfectly explicit, the variational form for the momentum equation is

obtained as follows. Letting $\phi_\rho = \phi_\sigma = 0$, we find

$$\begin{aligned}&(\phi_m, \partial_t m_h) + (m_h \partial_x u_h, \phi_m)_{L^2} - (m_h u_h, \partial_x \phi_m)_{L^2} \\ &+ (\rho_h \partial_x \eta_h, \phi_m)_{L^2} + (\sigma_h \partial_x T_h, \phi_m)_{L^2} + \frac{1}{\mathrm{Re}} (\partial_x u_h, \partial_x \phi_m)_{L^2} = 0\,, \quad \forall \phi_m \in V_h\,, \end{aligned} \tag{4.26}$$

where for all $(\phi_\eta, \phi_u, \phi_T) \in V_h^3$

$$\begin{aligned}&\left(\eta_h + \frac{m_h^2}{2\rho_h^2} - U\left(\rho_h, \frac{\sigma_h}{\rho_h}\right) - \rho_h \partial_1 U\left(\rho_h, \frac{\sigma_h}{\rho_h}\right) + \frac{\rho_h}{\sigma_h} \partial_2 U\left(\rho_h, \frac{\sigma_h}{\rho_h}\right), \phi_\eta\right)_{L^2} = 0\,, \\ &\left(u_h - \frac{m_h}{\rho_h}, \phi_u\right)_{L^2} = 0\,, \quad \text{and} \quad \left(T_h - \partial_2 U\left(\rho_h, \frac{\sigma_h}{\rho_h}\right), \phi_T\right)_{L^2} = 0\,. \end{aligned} \tag{4.27}$$

The continuity and entropy equations are obtained in a similar fashion.

As mentioned previously, the spatially semi-discretized evolution equations given in equation (4.19) are thermodynamically consistent. This may be verified by letting $\boldsymbol{v}_h = \delta \boldsymbol{h}_h$, yielding

$$\dot{H}^h = (\delta \boldsymbol{h}_h, \partial_t \boldsymbol{u}_h)_{L^2} = 0\,, \tag{4.28}$$

and $\boldsymbol{v}_h = \delta \boldsymbol{s}_h$, yielding

$$\dot{S}^h = (\delta \boldsymbol{s}_h, \partial_t \boldsymbol{u}_h)_{L^2} = \frac{1}{\mathrm{Re}} \left[\left(\frac{(\partial_x u_h)^2}{T_h}, 1 \right)_{L^2} + \frac{1}{\mathrm{Pr}} \frac{\gamma}{\gamma - 1} \left(\frac{(\partial_x T_h)^2}{T_h^2}, 1 \right)_{L^2} \right] \geq 0\,. \tag{4.29}$$

4.3.1 TEMPORAL DISCRETIZATION

One convenient and simple choice for temporal discretization is the implicit midpoint method. That is, for a differential equation $\dot{z} = V(z)$, its evolution is given by

$$\frac{z^{n+1} - z^n}{\Delta t} = V\left(\frac{z^{n+1} + z^n}{2}\right)\,. \tag{4.30}$$

This is done because the method is symplectic, A-stable, and known to preserve invariants well: quadratic invariants are preserved exactly [Hairer et al., 2013]. Mass is conserved exactly, and in the dissipation-free limit, so is entropy. The energy is not a polynomial invariant and therefore is not conserved exactly even in the dissipation-free limit. In fact, as the spatially semi-discrete model is not Hamil-

tonian even in the dissipation-free limit (although it does conserve energy due to antisymmetry of the Poisson bracket and degeneracy of the metriplectic bracket) there is no guarantee of the long-time near energy conservation property symplectic integrators usually enjoy [Hairer et al., 2013]. This is because the proof of long-time energy conservation for symplectic integrators applied to Hamiltonian systems crucially relies on the Hamiltonian structure, namely that the time-advance map is a canonical transformation. In fact, a small drift in energy is observed in the numerical results section in both the dissipation-free and dissipative test cases, see Figures 4.2(a) and 4.2(b) respectively. Entropy production of the fully discrete system is given by

$$\frac{S^{n+1}-S^n}{\Delta t} = \frac{1}{\mathrm{Re}}\left[\left(\frac{(\partial_x u_h^n)^2}{T_h^n},1\right)_{L^2} + \frac{1}{\mathrm{Pr}}\frac{\gamma}{\gamma-1}\left(\frac{(\partial_x T_h^n)^2}{(T_h^n)^2},1\right)_{L^2}\right] \geq 0\,. \tag{4.31}$$

The failure of the implicit midpoint method to yield a thermodynamically-consistent time-discretization motivates us to consider a time-stepping strategy based on the averaged vector-field discrete gradient method [Quispel and McLaren, 2008, Hairer, 2010]. The time-stepping method based on the averaged vector-field discrete gradient method for equation (4.19) is given by the weak form

$$\begin{aligned}\left(\frac{\boldsymbol{u}_h^{n+1}-\boldsymbol{u}_h^n}{\Delta t},\boldsymbol{v}_h\right)_{L^2} + \{\delta\boldsymbol{h}_h^n,\boldsymbol{v}_h\}\left(\frac{\boldsymbol{u}_h^{n+1}+\boldsymbol{u}_h^n}{2}\right) + (\delta\boldsymbol{s}_h^n,\boldsymbol{v}_h)_H(\delta\boldsymbol{h}_h^n)\\ + (\overline{DH}(\boldsymbol{u}_h^n,\boldsymbol{u}_h^{n+1}) - \delta\boldsymbol{h}_h^n,\boldsymbol{w}_h)_{L^2} = 0\,, \quad \forall(\boldsymbol{v}_h,\boldsymbol{w}_h)\in V_h^3\times V_h^3\end{aligned} \tag{4.32}$$

where

$$\overline{DH}(\boldsymbol{u}_h^n,\boldsymbol{u}_h^{n+1}) = \int_0^1 DH((1-t)\boldsymbol{u}_h^n + t\boldsymbol{u}_h^{n+1})\mathsf{d}t\,. \tag{4.33}$$

This method is equivalent to the implicit midpoint method if we approximate the integral in (4.33) using the midpoint rule. In fact, this integral must be approximated via quadrature in general. We find that Gauss-Legendre quadrature with ≥ 4 quadrature points achieves sufficient accuracy to achieve energy conservation to machine precision in the tests considered in this work. From this definition of the time-stepping scheme, it follows that if we let $\boldsymbol{v}_h = \delta\boldsymbol{h}_h$, then the fundamental

theorem of calculus implies that

$$\begin{aligned}\left(\frac{\boldsymbol{u}_h^{n+1}-\boldsymbol{u}_h^n}{\Delta t},\delta\boldsymbol{h}_h\right)_{L^2} &= \left(\frac{\boldsymbol{u}_h^{n+1}-\boldsymbol{u}_h^n}{\Delta t},\overline{DH}(\boldsymbol{u}_h^n,\boldsymbol{u}_h^{n+1})\right)_{L^2}\\ &= \frac{1}{\Delta t}\int_0^1 DH((1-t)\boldsymbol{u}_h^n+t\boldsymbol{u}_h^{n+1})\cdot(\boldsymbol{u}_h^{n+1}-\boldsymbol{u}_h^n)\mathsf{d}t\\ &= \frac{1}{\Delta t}\int_0^1 \frac{\mathsf{d}}{\mathsf{d}t}H((1-t)\boldsymbol{u}_h^n+t\boldsymbol{u}_h^{n+1})\mathsf{d}t = \frac{H(\boldsymbol{u}_h^{n+1})-H(\boldsymbol{u}_h^n)}{\Delta t}=0\,,\end{aligned} \tag{4.34}$$

verifying energy conservation. Positive entropy production follows from letting $\boldsymbol{v}_h = \delta\boldsymbol{s}_h^n$:

$$\begin{aligned}\frac{S^{n+1}-S^n}{\Delta t} &= (\delta\boldsymbol{s}_h^n,\delta\boldsymbol{s}_h^n)_H(\delta\boldsymbol{h}_h)\\ &= \frac{1}{\mathrm{Re}}\left[\left(\frac{(\partial_x u_h^n)^2}{T_h^n},1\right)_{L^2}+\frac{1}{\mathrm{Pr}}\frac{\gamma}{\gamma-1}\left(\frac{(\partial_x T_h^n)^2}{(T_h^n)^2},1\right)_{L^2}\right]\geq 0\,.\end{aligned}$$

Hence, the fully discrete method is found to be thermodynamically-consistent. This is verified in figures 4.2(c) and 4.2(d) for both the dissipation-free and dissipative test cases. The averaged vector field discrete gradient method is $O(\Delta t^2)$, however higher order generalizations were derived in [Cohen and Hairer, 2011]. Moreover, both the Gauss-Legendre implicit Runge-Kutta methods and energy conserving methods of the kind found in [Cohen and Hairer, 2011] were recently shown to fit into a general framework in [Andrews and Farrell, 2024].

4.4 NUMERICAL EXAMPLES

The spatial discretization is accomplished using the Firedrake library [Ham et al., 2023], and the temporal discretization with the Irksome module [Farrell et al., 2021]. For the finite element discretizations, we use piecewise linear interpolation. Although there is no inherent limitation which forces one to use linear finite elements, sharp gradients form in this compressible flow problem making it advantageous to use a fine grid with low order interpolation. In the following examples, we use the parameters

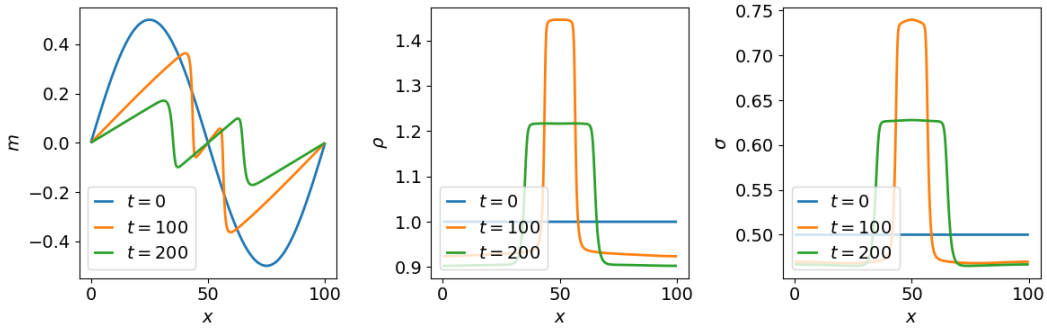
$$\mathrm{Re}=10\,,\quad \mathrm{Pr}=0.71\,,\quad \text{and}\quad \gamma=1.4 \tag{4.35}$$

to reflect the standard parameters of dry air with a relatively low Reynolds number (so that the effects of dissipation might be readily seen). We present two simulations with initial conditions $m_h(x,0) = \sin(2\pi x/L)/2$, $\rho_h(x,0) = 1$, and $\sigma_h(x,0) = 1/2$. In one simulation, we use the parameter set (4.35), in the other, we let $\mathrm{Re} \to \infty$ to simulate the dissipation-free dynamics (terminated prior to shock formation). The spatial domain is taken to be $[0, L] = [0, 100]$. Tests are run using both the implicit midpoint and discrete gradient time-stepping schemes. In all tests, the time step is taken to be $\Delta t = 0.1$, and the grid size is $\Delta x = L/2000 = 0.05$. For the dissipative simulations, the simulation is run for $t \in [0, 200]$, while the dissipation-free simulation is run for $t \in [0, 50]$ (due to the lack of viscous regularization, a shock forms at $t \approx 50$). See Figure 4.1 for a visualization of the simulation results, and Figure 4.2 for a visualization of the mass, energy, and entropy as a function of time for each simulation.

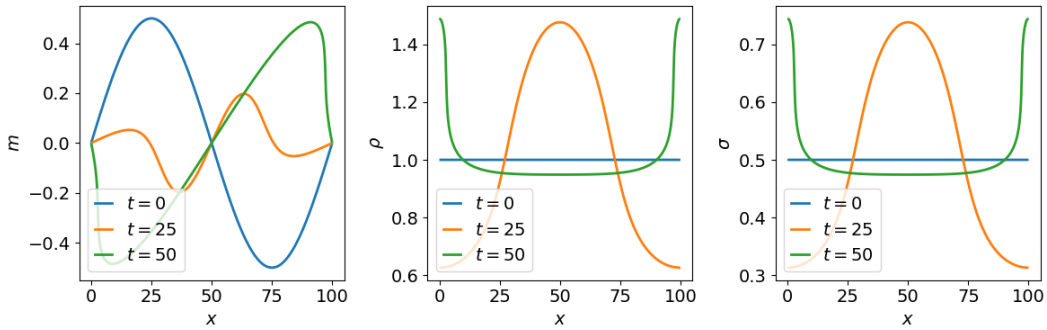
As previously mentioned, the implicit midpoint method fails to conserve energy whereas the discrete gradient method does, as seen in Figure 4.2. Because the dissipation-free system is not Hamiltonian, there is no guarantee that a symplectic integrator should enjoy long-time energy conservation. However, even if the dissipation-free spatially discrete system were Hamiltonian—so that symplectic integration yielded a long-time energy near-conservation result—proving energy conservation for the fully-discrete metriplectic system remains problematic. The conserved modified energy obtained through backward error analysis would most likely fail to lie in the null space of the metriplectic bracket. Thus, overall energy conservation of the coupled conservative-dissipative dynamics remains uncertain even in this optimistic case. For these reasons, symplectic integration is not an appropriate choice for the time-integration of metriplectic systems. Rather, energy conserving methods—such as the averaged vector field discrete gradient method used in this work—are more appropriate.

4.5 DISCUSSION AND CONCLUSION

In this short chapter, we derived a thermodynamically consistent discretization of the one dimensional Navier-Stokes-Fourier model using the metriplectic 4-bracket formalism. For Galerkin methods, one simply restricts the brackets and functionals to act on finite dimensional function spaces. A comparable discretization using finite-differences could be derived by directly approximating the functionals and brackets using quadrature. Virtually any spatial discretization method, if applied at the level



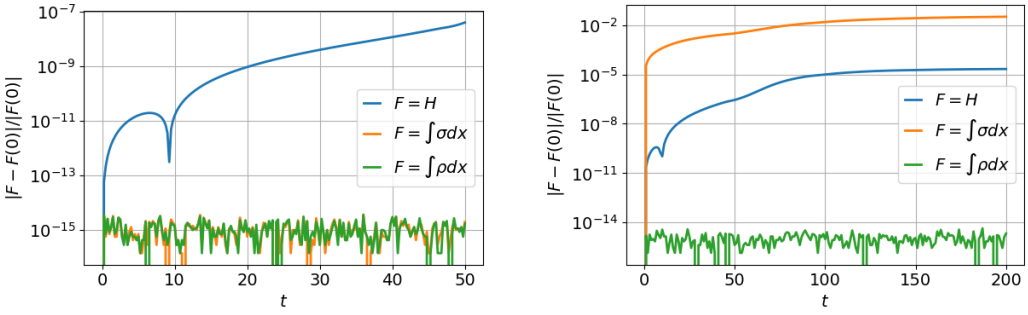
(a) Re = 10



(b) Re = ∞

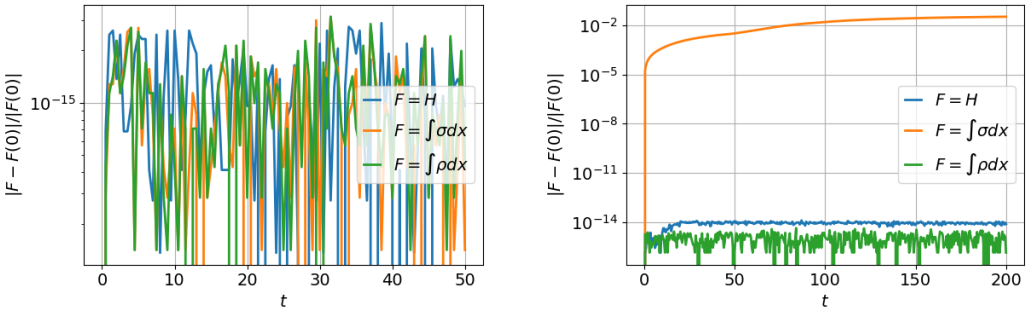
Figure 4.1: Visualization of solutions. The dissipation-free solution is shown prior to shock formation at $t \approx 50$. The results using implicit midpoint and discrete-gradient time-stepping look indistinguishable to the eye.

of the brackets and generating functions, would yield a thermodynamically consistent spatial semi-discretization as long as the resulting discrete brackets retain the symmetries and degeneracies of the continuous formulation. Many other models fit into the metriplectic formalism [Morrison and Updike, 2023, Zaidni et al., 2024, Sato and Morrison, 2024], and one may reasonably expect their discretization to likewise be thermodynamically consistent if one uses analogous methods to those employed in this paper. The implicit midpoint method was found to yield largely favorable behavior as a time-integrator, however it fails to exactly conserve energy. The averaged vector field discrete gradient method [Hairer, 2010, McLachlan et al., 1999] applied to the bracket-based spatial discretization yielded a thermodynamically consistent fully-discrete method. Other energy-conserving methods such as those found in [Cohen and Hairer, 2011, Andrews and Farrell, 2024] could likewise be used. The simultaneous guarantee of energy conservation and the positive production of phys-



(a) Re $= \infty$ with implicit midpoint time-stepping.

(b) Re $= 10$ with implicit midpoint time-stepping.



(c) Re $= \infty$ with discrete gradient time-stepping.

(d) Re $= 10$ with discrete gradient time-stepping.

Figure 4.2: Evolution of relative error in total energy, entropy, and mass.

ical entropy at the correct rate makes these energy-conserving methods preferable to standard time-stepping methods. Finally, compressible flow models exhibit discontinuous shock solutions in the inviscid case, and effective shocks if the spatial discretization does not resolve the viscous boundary layer. A thermodynamically consistent spatial discretization based on a discontinuous Galerkin, finite volume, or finite difference method with stabilization for shock solutions using the metriplectic formalism is an intriguing future direction of inquiry.

Previously, 2-brackets have been used and proposed in [Kraus and Hirvijoki, 2017, Hirvijoki et al., 2018, Bressan et al., 2018, Gruber et al., 2023, Jeyakumar et al., 2024] to obtain thermodynamically consistent numeric, i.e., where the semi-discrete equations are a finite-dimensional metriplectic system in terms of the 2-bracket. However, the 4-bracket was found to be particularly useful because maintaining symmetries while projecting onto a Galerkin basis is essentially automatic.

CHAPTER

WELL-POSEDNESS ANALYSIS OF CHNS SYSTEM 5

5.1 INTRODUCTION

In this chapter, We study the well-posedness of anisotropic, incompressible Cahn-Hilliard-Navier-Stokes system derived from Sec. 3.4.3 (for the case $a = 0$ (3.160)–(3.162)). This extends previous studies on the isotropic case by incorporating the anisotropic surface energy, represented by $\mathfrak{F} = \int_\Omega \frac{\epsilon}{2}\Gamma^2(\nabla\phi)$. Using a Galerkin approximation scheme, we will prove the existence of global weak solutions in both two and three dimensions. Here, we adjust the notation to better accommodate readers familiar with PDEs analysis. In this case, the nonlinear system of equations governing the motion of a mixture of two incompressible non-Newtonian fluids is given by:

$$\partial_t\rho + \mathbf{u}\cdot\nabla\rho = 0, \tag{5.1}$$
$$\rho\partial_t\phi + \rho\mathbf{u}\cdot\nabla\phi = \operatorname{div}(D(\phi)\nabla\mu), \tag{5.2}$$
$$\rho\partial_t\mathbf{u} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} - \operatorname{div}(\nu(\phi)\mathbb{D}(\mathbf{u})) = -\nabla\pi - \operatorname{div}(\Gamma\boldsymbol{\zeta}(\nabla\phi)\otimes\nabla\phi), \tag{5.3}$$
$$\rho\mu = \rho F'(\phi) - \operatorname{div}(\Gamma\boldsymbol{\zeta}(\nabla\phi)), \tag{5.4}$$

where π the pressure, $\nu(\phi)$ the viscosity, $D(\phi)$ the diffusion coefficient, and μ the chemical potential. The symmetric strain-rate tensor of $\mathbf{u}$ is denoted by $\mathbb{D}(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u}+\nabla\mathbf{u}^T)$. The function F represents the logarithmic function defined on $[-1,1]$,

which follows from a mean-field model:

$$F(s) = \frac{\lambda_1}{2}(1-s^2) + \frac{\lambda_2}{2}\left[(1+s)\ln\frac{(1+s)}{2} + (1-s)\ln\frac{(1-s)}{2}\right] := \frac{\lambda_1}{2}(1-s^2) + G(s).$$

where $0 < \lambda_2 < \lambda_1$. As above, Γ is a homogeneous function of degree one of $\mathbf{p} = (p_1, \ldots, p_d) \in \mathbb{R}^d$, and $\boldsymbol{\zeta}$ is defined as:

$$\Gamma(\mathbf{p}) = \mathbf{p} \cdot \boldsymbol{\zeta} \coloneqq p_j \frac{\partial \Gamma(\mathbf{p})}{\partial p_j}.$$

The system is considered in $\Omega \times (0, T)$, where Ω is a bounded domain (open and connected set) in $\mathbb{R}^d$ for $d = 2, 3$, with a regular boundary $\partial\Omega$, and $T > 0$ is a given positive time.

We complete the system with the following initial conditions:

$$\rho(\cdot, 0) = \rho_0,\ \mathbf{u}(\cdot, 0) = \mathbf{u}_0,\ \phi(\cdot, 0) = \phi_0 \qquad \text{in } \Omega, \tag{5.5}$$

and one of the alternative boundary conditions:

- No-slip boundary condition for the velocity and homogeneous Neumann-Neumann boundary condition:

$$\mathbf{u} = 0,\ \partial_{\mathbf{n}}\mu = \partial_{\mathbf{n}}\phi = 0,\ \Gamma\boldsymbol{\zeta}(\nabla\phi)\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega \times (0, T) \tag{5.6}$$

- Dirichlet boundary condition:

$$\mathbf{u} = 0,\ \mu = \phi = 0, \qquad \text{on } \partial\Omega \times (0, T) \tag{5.7}$$

In the case of homogeneous Neumann-Neumann boundary condition (5.6), we make the following assumption

- $\mathbf{H}_0$: The Laplacian operator $\phi \mapsto \Delta\phi$ on $H^1(\Omega)$, with the zero Neumann-Neumann boundary conditions $\partial_{\mathbf{n}}\phi = 0,\ \Gamma\boldsymbol{\zeta}(\nabla\phi)\cdot\mathbf{n} = 0$ (cf. (5.6)) admits a basis of eigenfunctions $\{\omega_j\}_{j\geq 1}$.

Throughout this work, the functions $\nu(s)$ and $D(s)$ are assumed to be in $W^{1,\infty}(\mathbb{R})$ such that $0 < \nu_* \leq \nu \leq \nu^*$ and $0 < D_* \leq D \leq D^*$, where ν_*, ν^*, D_*, and D^* are positive constants.

Previous works primarily focused on the isotropic case. We present here a concise review of systems with variable density that have been studied in the literature.

The existence of global weak solutions for the incompressible Cahn-Hilliard-Navier-Stokes (CHNS) system with variable density has been established in both two and three dimensions Giorgini and Temam [2020], Abels et al. [2024], Munteanu [2024], Rui et al. [2024], Abels et al. [2013]. For results concerning strong solutions, we refer the reader to Zhao [2019], Li et al. [2024], Kotschote and Zacher [2015]. In the compressible case, results have been proven in one dimensional Chen et al. [2018], Cherfils et al. [2019], Elbar and Poulain [2024], Giorgini et al. [2021]. Beyond the isotropic case, the global existence of solutions for higher-order Navier-Stokes-Cahn-Hilliard systems in two dimensions has also been established Pan et al. [2020].

In this chapter, we prove the existence of global weak solutions for the incompressible anisotropic Cahn-Hilliard-Navier-Stokes system (5.1)-(5.4). To do this, let us state our assumptions regarding the anisotropic surface energy. We assume that the function Γ satisfies:

- $\mathbf{H}_1$: There exist two positive numbers, r and R, such that for any $\mathbf{p} \in \mathbb{R}^d$, we have $r\|\mathbf{p}\|_2^2 \leq \Gamma^2(\mathbf{p}) \leq R\|\mathbf{p}\|_2^2$, where $\|\mathbf{p}\|_2^2 = \sum_{i=1}^d p_i^2$.
- $\mathbf{H}_2$: The map $\mathbf{p} \mapsto \Gamma\boldsymbol{\zeta}(\mathbf{p})$ is linear.
- $\mathbf{H}_3$: The inner product $\mathbf{p} \cdot \Gamma\boldsymbol{\zeta}(\mathbf{p})$ is non-negative for any $\mathbf{p} \in \mathbb{R}^d$.

Taylor and Cahn [1998] provide a family of candidate functions Γ, specifically:

$$\Gamma^2_{\alpha,\beta}(\mathbf{p}) = p_1^2+p_2^2+p_3^2+2\alpha(|p_1p_2|+|p_1p_3|+|p_2p_3|)+2\beta(|p_1-p_2|^2+|p_1-p_3|^2+|p_2-p_3|^2),$$

for $d = 3$ and $\alpha, \beta > -1$. The functions $\Gamma_{\alpha,\beta}$ satisfy $\mathbf{H}_1$, $\mathbf{H}_2$, and $\mathbf{H}_3$ for $\alpha = 0$ and $\beta > -1/8$. A set of functions that satisfy the previous assumptions is provided by $\Gamma^2(\mathbf{p}) = \mathbf{p}^T\mathbf{M}\mathbf{p}$, where $\mathbf{M}$ is a positive definite matrix. In this case, R and r represent the largest and smallest eigenvalues of the matrix $\mathbf{M}$, respectively.

Here, we give an example where $\alpha = 0$ and $\beta = 1/2$. In this case, we have

$$\Gamma\boldsymbol{\zeta}(\nabla\phi)\otimes\nabla\phi = \begin{bmatrix} 3(\partial_x\phi)^2 - \partial_x\phi\partial_y\phi - \partial_x\phi\partial_z\phi & -(\partial_y\phi)^2 + 3\partial_x\phi\partial_y\phi - \partial_2\phi\partial_z\phi & -(\partial_z\phi)^2 - \partial_y\phi\partial_z\phi + 3\partial_x\phi\partial_z\phi \\ -(\partial_x\phi)^2 + 3\partial_x\phi\partial_y\phi - \partial_x\phi\partial_z\phi & 3(\partial_y\phi)^2 - \partial_x\phi\partial_y\phi - \partial_y\phi\partial_z\phi & -(\partial_z\phi)^2 + 3\partial_y\phi\partial_z\phi - \partial_y\phi\partial_z\phi \\ -(\partial_x\phi)^2 - \partial_x\phi\partial_y\phi + 3\partial_x\phi\partial_z\phi & -(\partial_y\phi)^2 - \partial_x\phi\partial_y\phi + 3\partial_2\phi\partial_z\phi & 3(\partial_z\phi)^2 - \partial_z\phi\partial_x\phi - \partial_z\phi\partial_y\phi \end{bmatrix} \tag{5.8}$$

The equation (5.4) then becomes

$$\rho\mu = \rho F'(\phi) - 3\Delta\phi - 2\partial_{xy}\phi - 2\partial_{xz}\phi - 2\partial_{yz}\phi. \tag{5.9}$$

5.2 GLOBAL EXISTENCE OF WEAK SOLUTIONS TO INCOMPRESSIBLE CHNS

Before formulating our main result, we need to introduce some definitions and notations. Let $\mathcal{C}_c^k(\Omega)$, $k \in \mathbb{N}$ be the space of all functions which, together with all partial derivatives up to order k, are continuous in Ω. Let $p \geq 1$ and $q > 0$. Then $L^p(\Omega)$ and $W^{q,p}(\Omega)$ are the usual Lebesgue and Sobolev spaces, respectively. $(f, g) := \int_\Omega f(x)g(x)\,dx$ denotes the scalar product with respect to the spatial variable. Moreover, for a Banach space X and a real interval I, we denote by $L^p(I; X)$ the Bochner space, which is equipped with the norm $\left(\int_I \|\,.\,\|_X^p\,dt\right)^{1/p}$.

We introduce the following velocity spaces

$$\mathfrak{C} = \left\{ \mathbf{u} \in \left(\mathcal{C}_c^\infty(\Omega)\right)^d \,;\, \operatorname{div} \mathbf{u} = 0 \right\},$$

$$\mathbf{V} = \text{the closure of } \mathfrak{C} \text{ in } \left(H_0^1(\Omega)\right)^d,$$

$$\mathbf{H} = \text{the closure of } \mathfrak{C} \text{ in } \left(L^2(\Omega)\right)^d,$$

where $\mathcal{C}_c^\infty(\Omega)$ is the space of smooth functions with compact support in Ω.

Given $1 \leq p \leq +\infty$, the Besov spaces denoted by $B^{\frac{1}{4}}_{p,\infty}(0,T;X)$ consist of the set of functions $f \in L^p(0,T;X)$ with finite norm

$$\|f\|_{B^{\frac{1}{4}}_{p,\infty}(0,T;X)} = \|f\|_{L^p(0,T;X)} + \sup_{0<h\leq 1} h^{-\frac{1}{4}} \|\Delta_h f\|_{L^p(I_h;X)},$$

where $\Delta_h f(t) = f(t+h) - f(t)$ and $I_h = \{t \in (0,T) : t + h \in (0,T)\}$.

We now state the main result of our paper as follows.

Theorem 1. *Let T be a positive time. Assume that $\rho_0 \in L^\infty(\Omega)$ with $0 < \rho_* \leq \rho_0 \leq \rho^* < \infty$, $\mathbf{u}_0 \in L^2(\Omega)$, and $\phi_0 \in H^1(\Omega) \cap L^\infty(\Omega)$ such that $\|\phi_0\|_{L^\infty(\Omega)} \leq 1$. With the initial conditions* (5.5)*, and taking as boundary conditions either;* (5.6)*, supplemented with the assumption $\boldsymbol{H}_0$, or alternatively* (5.7)*, and assuming $\boldsymbol{H}_1$, $\boldsymbol{H}_2$ and $\boldsymbol{H}_3$, then, there exists a weak solution $(\rho, \mathbf{u}, \phi, \mu)$ to the system* (5.1)-(5.4) *satisfying*

$$\rho \in \mathcal{C}([0,T]; L^2(\Omega)) \cap L^\infty(\Omega \times (0,T)) \cap W^{1,\infty}\left(0,T; H^{-1}(\Omega)\right), \tag{5.10}$$

$$\mathbf{u} \in L^2\left(0,T; \mathbf{V}\right) \cap B^{\frac{1}{4}}_{2,\infty}\left(0,T; \mathbf{H}\right), \tag{5.11}$$

$$\phi \in L^2\left(0,T; H^1(\Omega)\right) \cap B^{\frac{1}{4}}_{\infty,\infty}\left(0,T; L^2(\Omega)\right), \tag{5.12}$$

$$\mu \in L^2\left(0,T; H^1(\Omega)\right), \tag{5.13}$$

In the following we present the proof of Theorem 1 with the boundary condition (5.6) and the assumption $\mathbf{H}_0$. The case with the boundary condition (5.7) can be treated similarly. The proof is structured as follows. In Sect. 5.3, we derive the energy balance. In Sec. 5.4, we introduce a system with the regularized logarithmic potential, which is defined on $\mathbb{R}$ and parameterized by $\varepsilon \in \left(0, 1 - \sqrt{1 - \lambda_2/\lambda_1}\right)$. In Sec. 5.5, we establish, through a Galerkin scheme, the global existence of the solution to the system with the regularized logarithmic potential. The proof is divided into three steps:

- **Step 1**: We construct a linearized version of the system and prove the existence of a solution using the classical Cauchy-Lipschitz theorem. The solution is defined only on a local time interval $[0, T_0)$, where T_0 depends on the initial data.

- **Step 2**: By analyzing the mapping that uses the function we linearized around as input and yields the solution from the Cauchy-Lipschitz theorem as output, and applying Bihari's inequality [Bihari, 1956], we establish the existence of a small time interval $[0, \widetilde{T}]$ where both the input and output data remain well-defined.

- **Step 3**: We establish the regularity of the solution, and we show that the map from input data to output data has a Schauder fixed point. This argument follows the same approach used in [Giorgini and Temam, 2020].

At the end of Sec. 5.5, we prove that the fixed point cannot blow up near a given finite time T_0. In Sec. 5.6, we present the proof of the main result, which is

structured in two parts. First, we establish that the Galerkin approximation has a convergent subsequence, and its limit is a global weak solution of the system with the regularized logarithmic potential. Second, we prove uniform estimates, and by passing to the limit as $\varepsilon \to 0^+$, we obtain a weak solution of our system (5.1)-(5.4).

5.3 ENERGY BALANCE

In this section, we report the total energy balance. By multiplying (5.3) by $\mathbf{u}$ and integrating over Ω, we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho|\mathbf{u}|^2\mathrm{d}x + \int_\Omega \nu(\phi)|\mathbb{D}(\mathbf{u})|^2\mathrm{d}x = \int_\Omega -\operatorname{div}(\Gamma\boldsymbol{\zeta}\otimes\nabla\phi)\cdot\mathbf{u}\,\mathrm{d}x. \tag{5.14}$$

We have

$$\operatorname{div}(\Gamma\boldsymbol{\zeta}\otimes\nabla\phi) = \nabla\phi(\operatorname{div}(\Gamma\boldsymbol{\zeta})) + \Gamma\boldsymbol{\zeta}\cdot\nabla(\nabla\phi) = \nabla\phi(\operatorname{div}(\Gamma\boldsymbol{\zeta})) + \nabla\left(\frac{1}{2}\Gamma^2(\nabla\phi)\right). \tag{5.15}$$

Using (5.4), we find

$$\begin{aligned} -\operatorname{div}(\Gamma\boldsymbol{\zeta}\otimes\nabla\phi) &= \rho\mu\nabla\phi - \rho F'(\phi)\nabla\phi - \nabla\left(\frac{1}{2}\Gamma^2(\nabla\phi)\right) \\ &= \rho\mu\nabla\phi - \rho\nabla F(\phi) - \nabla\left(\frac{1}{2}\Gamma^2(\nabla\phi)\right). \end{aligned} \tag{5.16}$$

Assuming the boundary condition on $\mathbf{u}$ (5.6), the equation (5.14) becomes

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho|\mathbf{u}|^2\mathrm{d}x + \int_\Omega \nu(\phi)|\mathbb{D}(\mathbf{u})|^2\mathrm{d}x = \int_\Omega \rho\mu\mathbf{u}\cdot\nabla\phi - \rho\mathbf{u}\cdot\nabla F(\phi)\mathrm{d}x. \tag{5.17}$$

Multiplying (5.4) by $\partial_t\phi$ and integrating, we have

$$\begin{aligned} \int_\Omega \rho\mu\,\partial_t\phi &= -\int_\Omega \partial_t\phi\,\operatorname{div}(\Gamma\boldsymbol{\zeta})\mathrm{d}x + \int_\Omega \rho F'(\phi)\partial_t\phi\,\mathrm{d}x \\ &= \int_\Omega \Gamma\boldsymbol{\zeta}\cdot\partial_t\nabla\phi\mathrm{d}x + \int_\Omega \rho F'(\phi)\partial_t\phi\,\mathrm{d}x \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{2}\Gamma^2(\nabla\phi) + \rho F(\phi)\,\mathrm{d}x - \int_\Omega F(\phi)\partial_t\rho\,\mathrm{d}x. \end{aligned} \tag{5.18}$$

Here, we used the boundary conditions $\Gamma\boldsymbol{\zeta}(\nabla\phi)\cdot\mathbf{n} = 0$.

Multiplying (5.2) by μ and integrating, we find using the Newman boundary conditions on μ

$$\int_\Omega \rho\mu\partial_t\phi \,\mathrm{d}x + \int_\Omega \rho\mu\mathbf{u}\cdot\nabla\phi \,\mathrm{d}x + \int_\Omega D(\phi)|\nabla\mu|^2\mathrm{d}x = 0. \tag{5.19}$$

By combining (5.17), (5.18), and (5.19), we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{2}\rho|\mathbf{u}|^2 + \frac{1}{2}\Gamma^2(\nabla\phi) + \rho F(\phi)\,\mathrm{d}x + \int_\Omega \nu(\phi)|\mathbb{D}(\mathbf{u})|^2 + D(\phi)|\nabla\mu|^2\mathrm{d}x = 0. \tag{5.20}$$

Here, the Ginzburg–Landau energy $\int_\Omega \frac{1}{2}\Gamma^2(\nabla\phi) + \rho F(\phi)\,\mathrm{d}x$ describes an interfacial energy associated with the region where ϕ is not close to the minima of $F(\phi)$ and $\int_\Omega \frac{1}{2}\rho|\mathbf{u}|^2\,\mathrm{d}x$ is the kinetic energy of the fluid.

5.4 REGULARIZED LOGARITHMIC POTENTIAL

We introduce a family of regular potentials F_ε that approximate the logarithmic potential (5.1). For any $\varepsilon \in (0, 1-\sqrt{1-\lambda_2/\lambda_1})$, we define

$$F_\varepsilon(s) = \frac{\lambda_1}{2}(1-s^2) + G_\varepsilon(s), \tag{5.21}$$

where G_ε is defined by

$$G_\varepsilon(s) = \begin{cases} \sum_{j=0}^2 \frac{1}{j!}G^{(j)}(1-\varepsilon)[s-(1-\varepsilon)]^j & \text{for } s \geq 1-\varepsilon, \\ G(s) & \text{for } s \in [-1+\varepsilon, 1-\varepsilon], \\ \sum_{j=0}^2 \frac{1}{j!}G^{(j)}(-1+\varepsilon)[s-(-1+\varepsilon)]^j & \text{for } s \leq -1+\varepsilon. \end{cases} \tag{5.22}$$

We have $F_\varepsilon \in \mathcal{C}^2(\mathbb{R})$ and

$$F_\varepsilon(s) \leq F(s) \quad \text{for all } s \in (-1,1), \quad |F_\varepsilon'(s)| \leq |F'(s)| \quad \text{for all } s \in (-1,1). \tag{5.23}$$

In order to construct weak solutions by an approximation procedure, we intro-

duce the following regularized problem:

$$\partial_t \rho^\varepsilon + \mathbf{u}^\varepsilon \cdot \nabla \rho^\varepsilon = 0, \tag{5.24}$$

$$\rho^\varepsilon \partial_t \phi^\varepsilon + \rho^\varepsilon \mathbf{u}^\varepsilon \cdot \nabla \phi^\varepsilon = \operatorname{div}(D(\phi^\varepsilon)\nabla \mu^\varepsilon), \tag{5.25}$$

$$\rho^\varepsilon \partial_t \mathbf{u}^\varepsilon + \rho^\varepsilon (\mathbf{u}^\varepsilon \cdot \nabla^\varepsilon)\mathbf{u}^\varepsilon - \operatorname{div}(\nu(\phi^\varepsilon)\mathbb{D}(\mathbf{u}^\varepsilon)) = -\nabla \pi^\varepsilon - \operatorname{div}(\Gamma \xi(\nabla \phi^\varepsilon) \otimes \nabla \phi^\varepsilon), \tag{5.26}$$

$$\rho^\varepsilon \mu^\varepsilon = \rho^\varepsilon F'_\varepsilon(\phi^\varepsilon) - \operatorname{div}(\Gamma \xi(\nabla \phi^\varepsilon)). \tag{5.27}$$

Furthermore, we complete the system with the same boundary and initial conditions (5.6). The existence of weak solutions to the system (5.24)–(5.27) can be established by a standard argument: in the case of bounded domains, we construct approximate solutions via a Galerkin approximation scheme, derive uniform bounds, and thus obtain solutions by passing to the limit. This will be detailed in the next Sec. 5.5.

5.5 GLOBAL EXISTENCE OF APPROXIMATE SOLUTION

In this section, we construct a converging sequence using the Galerkin approximation scheme. We define the inner product on $\mathbf{V}$ by $(\mathbf{u}, \mathbf{v})_{\mathbf{V}} = (\nabla \mathbf{u}, \nabla \mathbf{v})$ and the norm $\|\mathbf{u}\|_{\mathbf{V}} = \|\nabla \mathbf{u}\|_{L^2(\Omega)}$. For any integer $n \geq 1$, we define the finite-dimensional subspaces of $\mathbf{V}$ and $H^1(\Omega)$, respectively, by $\mathbf{V}_n = \operatorname{span}\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ and $H_n = \operatorname{span}\{\omega_1, \ldots, \omega_n\}$, where the families of functions $\{\mathbf{v}_j\}_{j\geq 1}$ and $\{\omega_j\}_{j\geq 1}$ represent the eigenfunctions of the Stokes operator (with zero Dirichlet boundary conditions) and Laplace operator (with zero Neumann boundary conditions and $\Gamma \boldsymbol{\zeta}(\nabla \phi) \cdot \mathbf{n} = 0$) (according to the assumption $\mathbf{H}_0$), respectively. We denote $(0 < \lambda_1^s \leq \lambda_2^s \leq \ldots)$ and $(\lambda_1 \leq \lambda_2 \leq \ldots)$ as the corresponding eigenvalues of the Stokes operator and Laplace operator, respectively. We denote by P_n^1 and P_n^2 the orthogonal projections onto $\mathbf{V}_n$ and H_n with respect to the inner product in $\mathbf{H}$ and $L^2(\Omega)$, respectively. We define the initial data as follows: we consider the triplet $(\rho_{0n}, \mathbf{u}_{0n}, \phi_{0n})$, where $\mathbf{u}_{0n} = P_n^1 \mathbf{u}_0$ and $\phi_{0n} = P_n^2 \phi_0$, and ρ_{0n} constructed using mollification by convolution such that for any $n \geq 1$, $\rho_{0n} \in \mathcal{C}^\infty(\overline{\Omega})$ and $\rho_* \leq \rho_{0n}(x) \leq \rho^*$ for any $x \in \overline{\Omega}$. The constructed initial data satisfy

$$\rho_{0n} \to \rho_0 \quad \text{strongly in } L^2(\Omega), \tag{5.28}$$

$$\rho_{0n} \rightharpoonup \rho_0 \quad \text{weak-star in } L^\infty(\Omega), \tag{5.29}$$

$$\mathbf{u}_{0n} \to \mathbf{u}_0 \quad \text{strongly in } (L^2(\Omega))^d, \tag{5.30}$$

$$\phi_{0n} \to \phi_0 \quad \text{strongly in } H^1(\Omega). \tag{5.31}$$

We have $\mathbf{u}_{0n} = 0, \quad \partial_{\mathbf{n}}\mu_{0n} = \partial_{\mathbf{n}}\phi_{0n} = 0,$ on $\partial\Omega \times (0,T)$. Since $\Gamma\boldsymbol{\zeta}$ is linear, we also have

$$\Gamma\boldsymbol{\zeta}(\nabla\phi_{0n}) \cdot \mathbf{n} = \sum_{i=1}^{n} (\phi_{0n}, \omega_i)_{L^2(\Omega)} \Gamma\boldsymbol{\zeta}(\nabla\omega_i) \cdot \mathbf{n} = 0.$$

We recall that, for any $\mathbf{u}_n \in \mathbf{V}_n$ and $\phi_n \in H_n$, we have

$$\|\mathbf{u}_n\|_{L^2(\Omega)} \leq \frac{1}{\sqrt{\lambda_1^s}} \|\nabla\mathbf{u}_n\|_{L^2(\Omega)}, \tag{5.32}$$

$$\|\mathbf{u}_n\|_{\mathbf{V}} \leq \sqrt{\lambda_n^s} \|\mathbf{u}_n\|_{L^2(\Omega)}, \tag{5.33}$$

$$\|\phi_n\|_{H^2(\Omega)} \leq \sqrt{\lambda_n} \|\phi_n\|_{H^1(\Omega)}, \tag{5.34}$$

$$\|\mathbf{u}_n\|_{L^\infty(\Omega)} \leq K \|\mathbf{u}_n\|_{H^2(\Omega)} \leq K_n \|\mathbf{u}_n\|_{L^2(\Omega)}, \tag{5.35}$$

where K and K_n are constants. Let $1 \leq p \leq +\infty$.

Proposition 1. *(Local existence of approximate solution). Given the initial data $(\rho_{0n}, \mathbf{u}_{0n}, \phi_{0n}, \mu_{0n})$ constructed as above, there exist a time interval $[0, \widetilde{T}]$ with $\widetilde{T} > 0$ and $(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon, \mu_n^\varepsilon)$ such that*

$$\rho_n^\varepsilon \in \mathcal{C}^1(\bar{\Omega} \times [0,\widetilde{T}]), \ \mathbf{u}_n^\varepsilon \in \mathcal{C}^1([0,\widetilde{T}]; \mathbf{V}_n), \ \phi_n^\varepsilon \in \mathcal{C}^1([0,\widetilde{T}]; H_n), \ \mu_n^\varepsilon \in \mathcal{C}([0,\widetilde{T}]; H_n), \tag{5.36}$$

$$\partial_t \rho_n^\varepsilon + \mathbf{u}_n^\varepsilon \cdot \nabla\rho_n^\varepsilon = 0 \text{ in } \Omega \times (0,\widetilde{T}), \tag{5.37}$$

$$\begin{aligned}(\rho_n^\varepsilon \partial_t \mathbf{u}_n^\varepsilon, \mathbf{v}) + (\rho_n^\varepsilon (\mathbf{u}_n^\varepsilon \cdot \nabla)\mathbf{u}_n^\varepsilon, \mathbf{v}) + (\nu(\phi_n^\varepsilon)\mathbb{D}\mathbf{u}_n^\varepsilon, \nabla\mathbf{v}) =& (\rho_n^\varepsilon \mu_n^\varepsilon \nabla\phi_n^\varepsilon, \mathbf{v}) \\ &- (\rho_n^\varepsilon \nabla(F_\varepsilon(\phi_n^\varepsilon)), \mathbf{v}),\end{aligned} \tag{5.38}$$

$$(\rho_n^\varepsilon \partial_t \phi_n^\varepsilon, \omega) + (\rho_n^\varepsilon \mathbf{u}_n^\varepsilon \cdot \nabla\phi_n^\varepsilon, \omega) + (D(\phi_n^\varepsilon)\nabla\mu_n^\varepsilon, \nabla\omega) = 0, \tag{5.39}$$

$$(\rho_n^\varepsilon \mu_n^\varepsilon, \omega) = (\Gamma\boldsymbol{\zeta}(\nabla\phi_n^\varepsilon), \nabla\omega) + (\rho_n^\varepsilon F_\varepsilon'(\phi_n^\varepsilon), \omega), \tag{5.40}$$

for all $\mathbf{v} \in \mathbf{V}_n$, $\omega \in H_n$ and for all $t \in [0,\widetilde{T}]$.

One of the key steps in proving this proposition is the use of Bihari's inequality. [Bihari, 1956, see page 90] .

Lemma 3. *Let $h : [0,+\infty[\to [0,+\infty[$ be a non-decreasing continuous function such that $h > 0$ on $]0,+\infty[$ and $\int_1^{+\infty} \frac{1}{h(x)}\,dx < +\infty$. We denote the antiderivative of $-1/h$, which cancels at $+\infty$, as H. Let y be a continuous function that is nonnegative on $[0,+\infty[$, and let g be a nonnegative function in $L^1_{loc}([0,+\infty[)$. We assume that there exists a $y_0 > 0$ such that for all $t \geq 0$, we have the inequality*

$$y(t) \leq y_0 + \int_0^t g(s)\,ds + \int_0^t h(y(s))\,ds.$$

Then, there exists a unique T^* that satisfies the equation

$$T^* = H\left(y_0 + \int_0^{T^*} g(s)\,ds\right),$$

and for any $T < T^*$, we have

$$\sup_{t\le T} y(t) \le H^{-1}\left(H\left(y_0 + \int_0^{T} g(s)\,ds\right) - T\right).$$

Proof of the Proposition 1. **Step 1**: For any $n \ge 1$, let fix $(\widetilde{\mathbf{u}}_n^\varepsilon, \widetilde{\phi}_n^\varepsilon)$ such that $\widetilde{\mathbf{u}}_n \in \mathcal{C}([0,T];\mathbf{V}_n)$ and $\widetilde{\phi}_n^\varepsilon \in \mathcal{C}([0,T];H_n)$. The density function corresponding to the given velocity $\widetilde{\mathbf{u}}_n^\varepsilon$ is determined explicitly as

$$\rho_n^\varepsilon(x,t) = \rho_{0n}(\widetilde{y}_n^\varepsilon(0,t,x)), \quad \rho_n^\varepsilon \in \mathcal{C}^1(\bar{\Omega}\times[0,T]), \tag{5.41}$$

where $\widetilde{y}_n^\varepsilon$ is the unique solution of the following Cauchy problem

$$\frac{\mathrm{d}\widetilde{y}_n^\varepsilon}{\mathrm{d}\tau}(\tau,t,x) = \widetilde{\mathbf{u}}_n^\varepsilon(\widetilde{y}_n^\varepsilon(\tau,t,x),\tau), \qquad \widetilde{y}_n^\varepsilon(t,t,x) = x. \tag{5.42}$$

We have the following estimates

$$\rho_* \le \rho_n^\varepsilon(x,t) \le \rho^* \text{ for any } (x,t)\in\bar{\Omega}\times[0,T], \tag{5.43}$$

$$\max_{t\in[0,T]} \|\nabla\rho_n^\varepsilon(t)\|_{L^\infty(\Omega)} \le K\|\nabla\rho_{0n}\|_{L^\infty(\Omega)} \exp\left(\int_0^T \|\widetilde{\mathbf{u}}_n^\varepsilon(\tau)\|_{W^{1,\infty}(\Omega)}\mathrm{d}\tau\right), \tag{5.44}$$

where the constant K is independent of the integer n. Given a triplet $(\mathbf{u}_n, \phi_n, \mu_n)$ such that

$$\mathbf{u}_n^\varepsilon(x,t) = \sum_{i=1}^n \alpha_i^\varepsilon(t)\mathbf{v}_i(x), \quad \phi_n^\varepsilon(x,t) = \sum_{i=1}^n \beta_i^\varepsilon(t)\omega_i(x), \quad \mu_n^\varepsilon(x,t) = \sum_{i=1}^n \gamma_i^\varepsilon(t)\omega_i(x),$$

which solves the following system

$$\begin{aligned}(\rho_n^\varepsilon\partial_t\mathbf{u}_n^\varepsilon, \mathbf{v}_i) + (\rho_n^\varepsilon(\widetilde{\mathbf{u}}_n^\varepsilon\cdot\nabla)\mathbf{u}_n^\varepsilon, \mathbf{v}_i) + (\nu(\widetilde{\phi}_n^\varepsilon)\mathbb{D}\mathbf{u}_n^\varepsilon, \nabla\mathbf{v}_i) =& (\rho_n^\varepsilon\mu_n^\varepsilon\nabla\widetilde{\phi}_n^\varepsilon, \mathbf{v}_i)\\ &- (\rho_n^\varepsilon\nabla(F_\varepsilon(\phi_n^\varepsilon)), \mathbf{v}_i),\end{aligned} \tag{5.45}$$

$$(\rho_n^\varepsilon\partial_t\phi_n^\varepsilon, \omega_i) + (\rho_n^\varepsilon\mathbf{u}_n^\varepsilon\cdot\nabla\widetilde{\phi}_n^\varepsilon, \omega_i) + (D(\widetilde{\phi}_n^\varepsilon)\nabla\mu_n^\varepsilon, \nabla\omega_i) = 0, \tag{5.46}$$

$$(\rho_n^\varepsilon \mu_n^\varepsilon, \omega_i) = (\Gamma \boldsymbol{\zeta}(\nabla \phi_n^\varepsilon), \nabla \omega_i) + (\rho_n^\varepsilon F_\varepsilon'(\phi_n^\varepsilon), \omega_i), \tag{5.47}$$

for all $i = 1, \dots, N$.

We define the unknown multi-components quantities as follow $\mathbf{A}^n = (\alpha_1^\varepsilon, \dots, \alpha_n^\varepsilon)$, $\mathbf{B}^n = (\beta_1^\varepsilon, \dots, \beta_n^\varepsilon)$ and $\mathbf{C}^n = (\gamma_1^\varepsilon, \dots, \gamma_n^\varepsilon)$. Hence, we get from the classical Cauchy-Lipschitz theorem the existence and uniqueness of a maximal solution $(\mathbf{A}^n, \mathbf{B}^n) \in \mathcal{C}^1([0, T_0); \mathbb{R}^n \times \mathbb{R}^n), \mathbf{C}^n \in \mathcal{C}([0, T_0); \mathbb{R}^n)$.

Step 2: Let us multiply (5.45) by α_i^ε and summing over i, we find

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \frac{1}{2} \rho_n^\varepsilon |\mathbf{u}_n^\varepsilon|^2 \mathrm{d}x + \int_\Omega \nu(\widetilde{\phi}_n^\varepsilon) |\mathbb{D}(\mathbf{u}_n^\varepsilon)|^2 \mathrm{d}x = \int_\Omega \rho_n^\varepsilon \mu_n^\varepsilon \mathbf{u}_n^\varepsilon \cdot \nabla \widetilde{\phi}_n^\varepsilon \mathrm{d}x \\ - \int_\Omega \rho_n^\varepsilon \mathbf{u}_n \cdot \nabla F_\varepsilon(\phi_n^\varepsilon) \mathrm{d}x. \end{aligned} \tag{5.48}$$

Here the density is the solution to the transport equation with velocity $\widetilde{\mathbf{u}}_n^\varepsilon$. Now, we multiply (5.46) by γ_i^ε and (5.47) by $\frac{\mathrm{d}}{\mathrm{d}t}\beta_i^\varepsilon$, respectively, and summing over i, we get

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \left[\frac{1}{2} \Gamma^2 (\nabla \phi_n^\varepsilon) + \rho_n^\varepsilon F_\varepsilon(\phi_n^\varepsilon) \right] \mathrm{d}x + \int_\Omega D(\widetilde{\phi}_n^\varepsilon) |\nabla \mu_n^\varepsilon|^2 \mathrm{d}x + \int_\Omega \rho_n^\varepsilon \mathbf{u}_n^\varepsilon \cdot \nabla \widetilde{\phi}_n^\varepsilon \mu_n^\varepsilon \mathrm{d}x \\ = \int_\Omega \partial_t \rho_n^\varepsilon F_\varepsilon(\phi_n^\varepsilon) \mathrm{d}x \end{aligned} \tag{5.49}$$

By summing the two previous equation (5.48) and (5.49), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} E^\varepsilon(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon) + \int_\Omega \nu(\widetilde{\phi}_n^\varepsilon) |\mathbb{D}\mathbf{u}_n^\varepsilon|^2 + D(\widetilde{\phi}_n^\varepsilon) |\nabla \mu_n^\varepsilon|^2 = \mathcal{R}^\varepsilon, \tag{5.50}$$

where E^ε and $\mathcal{R}^\varepsilon$ are given by

$$E^\varepsilon(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon) = \int_\Omega \frac{1}{2} \rho_n^\varepsilon |u_n^\varepsilon|^2 + \frac{1}{2} \Gamma^2 (\nabla \phi_n^\varepsilon) + \rho_n^\varepsilon F_\varepsilon(\phi_n^\varepsilon) \, \mathrm{d}x, \tag{5.51}$$

$$\mathcal{R}^\varepsilon = \int_\Omega F_\varepsilon(\phi_n^\varepsilon)(\mathbf{u}_n^\varepsilon - \widetilde{\mathbf{u}}_n^\varepsilon) \cdot \nabla \rho_n^\varepsilon \, \mathrm{d}x. \tag{5.52}$$

We note that $\mathcal{R}^\varepsilon$ will be zero at the fixed point. Using (5.35) we get

$$\|\widetilde{\mathbf{u}}_n^\varepsilon\|_{\mathcal{C}([0,T];H^2(\Omega))} \leq K_n \|\widetilde{\mathbf{u}}_n^\varepsilon\|_{\mathcal{C}([0,T];L^2(\Omega))} \leq K_n K_0. \tag{5.53}$$

According to (5.44) and the fact that $H^3(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$, we have

$$\begin{aligned}\max_{t\in[0,T]} \|\nabla\rho_n(t)^\varepsilon\|_{L^\infty(\Omega)} &\le K\|\nabla\rho_{0n}\|_{L^\infty(\Omega)} \exp\left(\int_0^T K_1\|\widetilde{\mathbf{u}}_n^\varepsilon(\tau)\|_{H^3(\Omega)}\mathrm{d}\tau\right) \\ &\le K\|\nabla\rho_{0n}\|_{L^\infty(\Omega)} \exp\left(K_1K_nK_0T\right) := K_\rho.\end{aligned} \tag{5.54}$$

Here, the last inequality comes from the regularity theory of the Stokes operator

$$\|\widetilde{u_n}\|_{C([0,T];H^3(\Omega))} \le C(n)\|\widetilde{u_n}\|_{C([0,T];L^2(\Omega))} \qquad \forall\ \widetilde{u_n} \in \mathbf{V}_n.$$

Next, we have $F_\varepsilon(s) \ge 0$ for all s in $\mathbb{R}$, then we control the quantity $\mathcal{R}^\varepsilon$ as follows

$$\begin{aligned}|\mathcal{R}^\varepsilon| &\le \frac{1}{\rho_*}\left(\int_\Omega \rho_n^\varepsilon F_\varepsilon(\phi_n^\varepsilon)\mathrm{d}x\right)\|\widetilde{\mathbf{u}}_n^\varepsilon - \mathbf{u}_n^\varepsilon\|_{L^\infty(\Omega)}\|\nabla\rho_n^\varepsilon\|_{L^\infty(\Omega)} \\ &\le \frac{K_nK_\rho}{\rho_*}E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon)\|\widetilde{\mathbf{u}}_n^\varepsilon - \mathbf{u}_n^\varepsilon\|_{L^2(\Omega)} \\ &\le \frac{K_nK_\rho}{\rho_*}E(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon)\|\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)} + \frac{K_nK_\rho K_0}{\rho_*}E(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon) \\ &\le \frac{K_nK_\rho}{\rho_*}E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon)\frac{\|\nabla\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}}{\sqrt{\lambda_1^s}} + \frac{K_nK_\rho K_0}{\rho_*}E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon) \\ &\le \frac{K_nK_\rho}{\rho_*}E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon)\frac{\sqrt{2}\sqrt{\nu_*}\|\mathbb{D}\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}}{\sqrt{\nu_*\lambda_1^s}} + \frac{K_nK_\rho K_0}{\rho_*}E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon) \\ &\le \int_\Omega \frac{\nu(\phi_n^\varepsilon)}{2}|\mathbb{D}\mathbf{u}_n^\varepsilon|^2\mathrm{d}x + \frac{K_n^2K_\rho^2}{\nu_*\rho_*^2\lambda_1^s}[E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon)]^2 + \frac{K_nK_\rho K_0}{\rho_*}E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon) \\ &\le \int_\Omega \frac{\nu(\phi_n^\varepsilon)}{2}|\mathbb{D}\mathbf{u}_n^\varepsilon|^2\mathrm{d}x + \frac{2K_n^2K_\rho^2}{\nu_*\rho_*^2\lambda_1^s}[E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon)]^2 + \frac{\nu_*\lambda_1^sK_0^2}{4}\end{aligned} \tag{5.55}$$

According to (5.50), we arrive at

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon) + \int_\Omega \frac{\nu(\phi_n^\varepsilon)}{2}|\mathbb{D}\mathbf{u}_n^\varepsilon|^2\mathrm{d}x + \int_\Omega D(\widetilde{\phi}_n^\varepsilon)|\nabla\mu_n^\varepsilon|^2\mathrm{d}x \le C_1[E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon)]^2 \\ + C_2K_0^2\end{aligned} \tag{5.56}$$

where $C_1 := 2K_n^2K_\rho^2/\nu_*\rho_*^2\lambda_1^s$ and $C_2 := \nu_*\lambda_1^s/4$. In particular, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon) \le C_1[E^\varepsilon(\rho_n^\varepsilon,\mathbf{u}_n^\varepsilon,\phi_n^\varepsilon)]^2 + C_2K_0^2. \tag{5.57}$$

Integrating over $[0,t]$ for $t < T_0$, we get

$$E^\varepsilon(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon)(t) \leq E^\varepsilon(\rho_{0n}, \mathbf{u}_{0n}, \phi_{0n}) + \int_0^t C_2 K_0^2 \mathrm{d}\tau + C_1 \int_0^t [E^\varepsilon(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon)(\tau)]^2 \mathrm{d}\tau, \tag{5.58}$$

where

$$E^\varepsilon(\rho_{0n}, \mathbf{u}_{0n}, \phi_{0n}) = \int_\Omega \frac{1}{2}\rho_{0n}|u_{0n}|^2 + \frac{1}{2}\Gamma^2(\nabla\phi_{0n}) + \rho_{0n}F_\varepsilon(\phi_{0n})\mathrm{d}x. \tag{5.59}$$

Now, we apply Bihari's inequality 3, with the following choice

$$y(t) = E^\varepsilon(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon)(t), \quad y_0 = E^\varepsilon(\rho_{0n}, \mathbf{u}_{0n}, \phi_{0n}) := E_n^\varepsilon(0), \tag{5.60}$$

$$g(s) = C_2 K_0^2, \quad h(s) = C_1 s^2. \tag{5.61}$$

The anti-derivative of $-\frac{1}{h(s)}$ which cancels at $+\infty$ is $H(s) := \frac{1}{C_1 s}$. Since $H^{-1}(s) = H(s)$, the Bihari's inequality in our case reads

$$\sup_{t\leq T'} E^\varepsilon(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon)(t) \leq \frac{1}{C_1\left(\frac{1}{C_1(E_n^\varepsilon(0)+C_2K_0^2T')} - T'\right)}, \quad \text{for all } \ T' < \min(T_0, T^*), \tag{5.62}$$

where $T^* = \frac{1}{C_1(E_n^\varepsilon(0)+C_2T^*)}$. Let K_0 be sufficiently large such that $\|\mathbf{u}_{0n}\|_{L^2(\Omega)} + \|\phi_{0n}\|_{H^1(\Omega)} \leq K_0^2$. We aim to show that there exists a sufficiently small time $\widetilde{T} = \widetilde{T}(K_0)$ ($\widetilde{T} < \min(T_0, T^*)$) such that

$$\|\mathbf{u}_n\|_{\mathcal{C}([0,\widetilde{T}];L^2(\Omega))} + \|\phi_n\|_{\mathcal{C}([0,\widetilde{T}];H^1(\Omega))} \leq K_0^2. \tag{5.63}$$

To this end, we use that

$$\|\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}^2 \leq \frac{2}{\rho_*}E^\varepsilon(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon), \quad \|\nabla\phi_n^\varepsilon\|_{L^2(\Omega)}^2 \leq \frac{2}{r}E^\varepsilon(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon).$$

Since the function F_ε is polynomial of degree two on the domain $\{s \in \mathbb{R}\,;\, |s| \geq 1-\varepsilon\}$, there exist $c_\varepsilon > 0$ and $M_\varepsilon > 0$ such that

$$F_\varepsilon(s) > M_\varepsilon s^2 \qquad \text{for all } \ |s| > c_\varepsilon, \tag{5.64}$$

which implies that

$$\|\phi_n^\varepsilon\|^2_{L^2(\Omega)} = \int_{|\phi_n^\varepsilon|\leq c_\varepsilon} |\phi_n^\varepsilon|^2 \mathrm{d}x + \int_{|\phi_n^\varepsilon|\leq c_\varepsilon} |\phi_n^\varepsilon|^2 \mathrm{d}x \leq c_\varepsilon^2|\Omega| + \frac{1}{\rho_* M_\varepsilon}\int_\Omega \rho_n^\varepsilon F_\varepsilon(\phi_n^\varepsilon)\mathrm{d}x$$
$$\leq c_\varepsilon^2|\Omega| + \frac{1}{\rho_* M_\varepsilon} E^\varepsilon(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon). \tag{5.65}$$

Thus,

$$\|\mathbf{u}_n^\varepsilon\|_{\mathcal{C}([0,\widetilde{T}];L^2(\Omega))} + \|\phi_n^\varepsilon\|_{\mathcal{C}([0,\widetilde{T}];H^1(\Omega))} \leq \theta \sup_{t\leq\widetilde{T}} E(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon)(t) + c_\varepsilon^2|\Omega|$$
$$\leq \theta\left(\frac{E_n(0) + C_2K_0^2\widetilde{T}}{1 - C_1E_n(0)\widetilde{T} - C_1C_2K_0^2\widetilde{T}^2}\right) + c_\varepsilon^2|\Omega| \tag{5.66}$$

where $\theta := \max\left\{\frac{2}{\rho_*}, \frac{1}{\rho_* M_\varepsilon}, \frac{2}{r}\right\}$. The following condition should be satisfied

$$\theta\left(\frac{E_n^\varepsilon(0) + C_2K_0^2\widetilde{T}}{1 - C_1E_n^\varepsilon(0)\widetilde{T} - C_1C_2K_0^2\widetilde{T}^2}\right) + c_\varepsilon^2|\Omega| \leq K_0^2, \tag{5.67}$$

which can be written as

$$E_n^\varepsilon(0) + C_2K_0^2\widetilde{T} \leq \frac{1}{\theta}(K_0^2 - c_\varepsilon^2|\Omega|) - C_1E_n^\varepsilon(0)\frac{1}{\theta}(K_0^2 - c_\varepsilon^2|\Omega|)\widetilde{T} - C_1C_2K_0^2\frac{1}{\theta}(K_0^2 - c_\varepsilon^2|\Omega|)\widetilde{T}^2. \tag{5.68}$$

Since we can take $\widetilde{T} \leq 1$ the condition holds if

$$E_n^\varepsilon(0) + \left(C_2K_0^2 + C_1E_n^\varepsilon(0)\frac{1}{\theta}(K_0^2 - c_\varepsilon^2|\Omega|) + C_1C_2\frac{1}{\theta}K_0^2(K_0^2 - c_\varepsilon^2|\Omega|)\right)\widetilde{T}$$
$$\leq \frac{1}{\theta}(K_0^2 - c_\varepsilon^2|\Omega|). \tag{5.69}$$

Thus, by taking $E_n^\varepsilon(0) < \frac{1}{\theta}(K_0^2 - c_\varepsilon^2|\Omega|)$, there exists $\widetilde{T} = \widetilde{T}(K_0)$ sufficiently small such that the inequality (5.69) holds. We conclude that

$$\|\mathbf{u}_n^\varepsilon\|_{\mathcal{C}([0,\widetilde{T}];L^2(\Omega))} + \|\phi_n^\varepsilon\|_{\mathcal{C}([0,\widetilde{T}];H^1(\Omega))} \leq K_0^2. \tag{5.70}$$

For any set of parameters $(n, \varepsilon, \rho_*, \rho^*, E_n^\varepsilon(0), \nu_*, \rho_{0n})$, let now introduce the set

$$\mathcal{S}_n = \{(\mathbf{u}_n^\varepsilon, \phi_n^\varepsilon) \in \mathcal{C}([0,\widetilde{T}]; \mathbf{V}_n \times H_n) : \|\mathbf{u}_n^\varepsilon\|_{\mathcal{C}([0,\widetilde{T}];L^2(\Omega))} + \|\phi_n^\varepsilon\|_{\mathcal{C}([0,\widetilde{T}];H^1(\Omega))} \leq K_0^2\}.$$

Step 3: Next, we show that the derivatives of $\mathbf{u}_n^\varepsilon$ and ϕ_n^ε with respect time are also bounded on $[0,\widetilde{T}]$. Multiplying (5.45) by $\frac{\mathrm{d}}{\mathrm{d}t}\alpha_i^\varepsilon(t)$ and summing over i, we find

$$\begin{aligned}\rho_*\|\partial_t\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}^2 \leq & C\rho^*\|\widetilde{\mathbf{u}}_n^\varepsilon\|_{H^2(\Omega)}\|\nabla\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}\|\partial_t\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}+\nu^*\|\nabla\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}\|\nabla\partial_t\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}\\ &+C\rho^*\|\mu_n^\varepsilon\|_{L^2(\Omega)}\|\widetilde{\phi}_n^\varepsilon\|_{H^2(\Omega)}\|\nabla\partial_t\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}\\ &+\rho^*C\left(1+\|\phi_n^\varepsilon\|_{H^2(\Omega)}^4\right)\|\partial_t\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}.\end{aligned}.$$

We multiply (5.47) by $\gamma_i^\varepsilon(t)$ and sum over i, we find

$$\begin{aligned}\rho_*\|\mu_n^\varepsilon\|_{L^2(\Omega)}^2 &\leq \left(\rho^*\|F_\varepsilon'(\phi_n^\varepsilon)\|_{L^2(\Omega)}+\|\operatorname{div}(\Gamma\boldsymbol{\zeta}(\nabla\phi_n^\varepsilon)\|_{L^2(\Omega)}\right)\|\mu_n^\varepsilon\|_{L^2(\Omega)}\\ &\leq\left(C\rho^*\|\phi_n^\varepsilon\|_{H^1(\Omega)}^3+C\|\phi_n^\varepsilon\|_{H^2(\Omega)}\right)\|\mu_n^\varepsilon\|_{L^2(\Omega)}\\ &\leq\left(C\rho^*\|\phi_n^\varepsilon\|_{H^1(\Omega)}^3+C\lambda_n\|\phi_n^\varepsilon\|_{H^1(\Omega)}\right)\|\mu_n^\varepsilon\|_{L^2(\Omega)}.\end{aligned}$$

Thus,

$$\|\mu_n^\varepsilon\|_{L^2(\Omega)}\leq C_\mu, \tag{5.71}$$

where $C_\mu = C_\mu(n,\varepsilon,\rho_*,\rho^*,\lambda_n,K_0)$. We deduce that there exist a constant $K_1 = K_1(n,\varepsilon,\rho_*,\rho^*,\nu^*,K_0)$ such that

$$\max_{[0,\widetilde{T}]}\|\partial_t\mathbf{u}_n^\varepsilon(t)\|_{L^2(\Omega)}\leq K_1^2. \tag{5.72}$$

In a similar way, multiplying (5.46) by $\frac{\mathrm{d}}{\mathrm{d}t}\beta_i^\varepsilon$ and summing over i, we get

$$\rho_*\|\partial_t\phi_n^\varepsilon\|_{L^2(\Omega)}^2\leq\left(C\rho^*\sqrt{\lambda_n^s}\sqrt{\lambda_n}\|\mathbf{u}_n^\varepsilon\|_{L^2(\Omega)}\|\widetilde{\phi}_n^\varepsilon\|_{H^1(\Omega)}+D_*\lambda_n\|\mu_n^\varepsilon\|_{L^2(\Omega)}\right)\|\partial_t\phi_n^\varepsilon\|_{L^2(\Omega)}.$$

Then, there exists $K_2 = K_2\left(n,\varepsilon,\rho_*,\rho^*,K_0\right)$ such that

$$\max_{[0,\widetilde{T}]}\|\partial_t\phi_n^\varepsilon(t)\|_{L^2(\Omega)}\leq K_2^2.$$

Let us set $\widetilde{K}_0^2 = K_1^2+K_2^2$. We consider the subset $\widetilde{\mathcal{S}}_n$ of $\mathcal{S}_n$ defined as

$$\begin{aligned}\widetilde{\mathcal{S}}_n=\Big\{(\mathbf{v}_n^\varepsilon,\psi_n^\varepsilon)\in\mathcal{C}^1\left([0,\widetilde{T}];\mathbf{V}_n\times H_n\right):&\max_{[0,\widetilde{T}]}\|\mathbf{v}_n^\varepsilon(t)\|_{L^2(\Omega)}+\max_{[0,\widetilde{T}]}\|\psi_n^\varepsilon(t)\|_{H^1(\Omega)}\leq K_0^2,\\ &\max_{[0,\widetilde{T}]}\|\partial_t\mathbf{v}_n^\varepsilon(t)\|_{L^2(\Omega)}+\max_{[0,\widetilde{T}]}\|\partial_t\psi_n^\varepsilon(t)\|_{H^1(\Omega)}\leq\widetilde{K}_0^2\Big\}\end{aligned}$$

By the Ascoli-Arzelà theorem, the set $\widetilde{\mathcal{S}}_n$ is compact in $\mathcal{S}_n$. We consider the map Λ defined as

$$\Lambda : \mathcal{S}_n \longmapsto \widetilde{\mathcal{S}}_n, \qquad (\widetilde{\mathbf{u}}_n^\varepsilon, \widetilde{\phi}_n^\varepsilon) \longmapsto \Lambda(\widetilde{\mathbf{u}}_n^\varepsilon, \widetilde{\phi}_n^\varepsilon) := (\mathbf{u}_n^\varepsilon, \phi_n^\varepsilon).$$

We prove that Λ is a continuous map on $\mathcal{S}_n$. Let $(\mathbf{v}_n^{\varepsilon,m}, \psi_n^{\varepsilon,m})$ be a sequence of $\mathcal{S}_n$ such that $(\mathbf{v}_n^{\varepsilon,m}, \psi_n^{\varepsilon,m})_m \to (\mathbf{v}_n^\varepsilon, \psi_n^\varepsilon)$ on $\mathcal{C}^1\left([0,\widetilde{T}]; \mathbf{V}_n \times H_n\right)$ as $m \to \infty$. By the formula (5.41) we find $\rho_n^{\varepsilon,m}$ and ρ_n^ε in $\mathcal{C}^1([0,\widetilde{T}] \times \bar{\Omega})$ corresponding to $\mathbf{v}_n^{\varepsilon,m}$ and $\mathbf{v}_n^\varepsilon$, respectively. We consider $\delta\rho_n^\varepsilon = \rho_n^{\varepsilon,m} - \rho_n^\varepsilon$ which solves

$$\partial_t \delta\rho_n^\varepsilon + \mathbf{v}_n^{\varepsilon,m} \cdot \nabla \delta\rho_n^\varepsilon + (\mathbf{v}_n^{\varepsilon,m} - \mathbf{v}_n^\varepsilon) \cdot \delta\rho_n^\varepsilon = 0$$

We multiply by $|\delta\rho_n^\varepsilon|^{r-1}\delta\rho_n^\varepsilon$ and integrating over Ω, we get

$$\begin{aligned}
\int_\Omega \partial_t(|\delta\rho_n^\varepsilon|^r)\mathrm{d}x &= -\int_\Omega \mathbf{v}_n^{\varepsilon,m} \cdot \nabla(|\delta\rho_n^\varepsilon|^r)\mathrm{d}x - \int_\Omega (\mathbf{v}_n^{\varepsilon,m} - \mathbf{v}_n^\varepsilon)|\delta\rho_n^\varepsilon|^{r-2}\delta\rho_n^\varepsilon \nabla\rho_n^\varepsilon \mathrm{d}x. \\
&= -\int_\Omega (\mathbf{v}_n^{\varepsilon,m} - \mathbf{v}_n^\varepsilon)|\delta\rho_n^\varepsilon|^{r-2}\delta\rho_n^\varepsilon \nabla\rho_n^\varepsilon \mathrm{d}x \\
&\leq ||\mathbf{v}_n^{\varepsilon,m} - \mathbf{v}_n^\varepsilon||_{L^r(\Omega)} ||(\delta\rho_n^\varepsilon)^{r-1}||_{L^{\frac{r}{r-1}}(\Omega)} ||\nabla\rho_n^\varepsilon||_{L^\infty(\Omega)}. \\
&\leq ||\mathbf{v}_n^{\varepsilon,m} - \mathbf{v}_n^\varepsilon||_{L^r(\Omega)} (||(\delta\rho_n^\varepsilon)||_{L^r(\Omega)})^{r-1} ||\nabla\rho_n^\varepsilon||_{L^\infty(\Omega)}
\end{aligned}$$

we get

$$(||(\delta\rho_n^\varepsilon)||_{L^r(\Omega)})^{1-r} \int_\Omega \partial_t(|\delta\rho_n^\varepsilon|^r)\mathrm{d} \leq ||\mathbf{v}_n^{\varepsilon,m} - \mathbf{v}_n^\varepsilon||_{L^r(\Omega)} ||\nabla\rho_n^\varepsilon||_{L^\infty(\Omega)}$$

Since $\delta\rho_n^\varepsilon(.,0) = 0$, we get

$$\max_{[0,\widetilde{T}]} ||\delta\rho_n^\varepsilon||_{L^r(\Omega)} \leq C \int_0^{\widetilde{T}} ||\mathbf{v}_n^{\varepsilon,m} - \mathbf{v}_n^\varepsilon||_{L^r(\Omega)} \mathrm{d}t. \tag{5.73}$$

Where C is a constant independent of m. Thus, for any $r \geq 2$, $\rho_n^{\varepsilon,m} \to \rho_n^\varepsilon$ strongly in $\mathcal{C}([0,\widetilde{T}]; L^r(\Omega))$.

We note $(\mathbf{u}_n^{\varepsilon,m}, \phi_n^{\varepsilon,m})$ and $(\mathbf{u}_n^\varepsilon, \phi_n^\varepsilon)$ the images by the map Λ of $(\mathbf{v}_n^{\varepsilon,m}, \psi_n^{\varepsilon,m})$ and $(\mathbf{v}_n^\varepsilon, \psi_n^\varepsilon)$, respectively.

$$\Lambda(\mathbf{v}_n^{\varepsilon,m}, \psi_n^{\varepsilon,m}) = (\mathbf{u}_n^{\varepsilon,m}, \phi_n^{\varepsilon,m}), \qquad \Lambda(\mathbf{v}_n^\varepsilon, \psi_n^\varepsilon) = (\mathbf{u}_n^\varepsilon, \phi_n^\varepsilon)$$

At the same way as above, there exist two K_1 and $\widetilde{K}_2$, depend on n, u_{0n}, ϕ_{0n} and

ρ_{0n} but independent of n such that the following estimates holds

$$\max_{[0,\widetilde{T}]}||\mathbf{u}_n^{\varepsilon,m}(t)||_{L^2(\Omega)}+\max_{[0,\widetilde{T}]}||\phi_n^{\varepsilon,m}(t)||_{H^1(\Omega)}\leq K_1^2, \tag{5.74}$$

$$\max_{[0,\widetilde{T}]}||\partial_t\mathbf{u}_n^{\varepsilon,m}(t)||_{L^2(\Omega)}+\max_{[0,\widetilde{T}]}||\partial_t\phi_n^{\varepsilon,m}(t)||_{H^1(\Omega)}\leq \widetilde{K}_1^2. \tag{5.75}$$

By Ascoli-Arzelà theorem there exist a subsequence $(\mathbf{u}_n^{\varepsilon,m_k},\phi_n^{\varepsilon,m_k})$ and (U,Φ) such that,

$$\mathbf{u}_n^{\varepsilon,m_k}\to U \text{ strongly in } \mathcal{C}([0,\widetilde{T}];\mathbf{V}_n),\quad \phi_n^{\varepsilon,m_k}\to\Phi \text{ strongly in } \mathcal{C}([0,\widetilde{T}];H_n)$$

$$\partial_t\mathbf{u}_n^{\varepsilon,m_k}\to\partial_t U \text{ weak-star in } L^\infty([0,\widetilde{T}];\mathbf{V}_n),\quad \partial_t\phi_n^{\varepsilon,m_k}\to\partial_t\Phi \text{ weak-star in } L^\infty([0,\widetilde{T}];H_n)$$

$$\mu_n^{\varepsilon,m_k}\to\Upsilon \text{ weakly in } L^2(0,\widetilde{T};H_n)$$

The equation $\Lambda(\mathbf{v}_n^{\varepsilon,m_k},\psi_n^{\varepsilon,m_k})=(\mathbf{u}_n^{\varepsilon,m_k},\phi_n^{\varepsilon,m_k})$ implies

$$\begin{aligned}(\rho_n^{\varepsilon,m_k}\partial_t\mathbf{u}_n^{\varepsilon,m_k},\mathbf{v}_i)+(\rho_n^{\varepsilon,m_k}(\mathbf{v}_n^{\varepsilon,m_k}\cdot\nabla)\mathbf{u}_n^{\varepsilon,m_k},\mathbf{v}_i)+(\nu(\psi_n^{\varepsilon,m_k})\mathbb{D}\mathbf{u}_n^{\varepsilon,m_k},\nabla\mathbf{v}_i)\\ =(\rho_n^{\varepsilon,m_k}\mu_n^{\varepsilon,m_k}\nabla\psi_n^{\varepsilon,m_k},\mathbf{v}_i)-(\rho_n^{\varepsilon,m_k}\nabla(F_\varepsilon(\phi_n^{\varepsilon,m_k})),\mathbf{v}_i),\end{aligned}$$

$$(\rho_n^{\varepsilon,m_k}\partial_t\phi_n^{\varepsilon,m_k},\omega_i)+(\rho_n^{\varepsilon,m_k}\mathbf{u}_n^{\varepsilon,m_k}\cdot\nabla\psi_n^{\varepsilon,m_k},\omega_i)+(D(\psi_n^{\varepsilon,m_k})\nabla\mu_n^{\varepsilon,m_k},\nabla\omega_i)=0,$$

$$(\rho_n^{\varepsilon,m_k}\mu_n^{\varepsilon,m_k},\omega_i)=(\Gamma\boldsymbol{\xi}(\nabla\phi_n^{\varepsilon,m_k}),\nabla\omega_i)+(\rho_n^{\varepsilon,m_k}F_\varepsilon'(\phi_n^{\varepsilon,m_k}),\omega_i).$$

For all $i=1,\dots,n$. We pass to the limit $m_k\to\infty$ in $\mathcal{D}'(0,\widetilde{T})$, we get

$$\begin{aligned}(\rho_n^{\varepsilon}\partial_t U,\mathbf{v}_i)+(\rho_n^{\varepsilon}(\mathbf{v}_n^{\varepsilon}\cdot\nabla)U,\mathbf{v}_i)+(\nu(\psi_n^{\varepsilon})\mathbb{D}U,\nabla\mathbf{v}_i)\\ =(\rho_n^{\varepsilon}\Upsilon\nabla\psi_n^{\varepsilon},\mathbf{v}_i)-(\rho_n^{\varepsilon}\nabla(F_\varepsilon(\Phi)),\mathbf{v}_i),\end{aligned}$$

$$(\rho_n^{\varepsilon}\partial_t\Phi,\omega_i)+(\rho_n^{\varepsilon}U\cdot\nabla\psi_n^{\varepsilon},\omega_i)+(D(\psi_n^{\varepsilon})\nabla\Upsilon,\nabla\omega_i)=0,$$

$$(\rho_n^{\varepsilon}\Upsilon,\omega_i)=(\Gamma\boldsymbol{\xi}(\nabla\Phi),\nabla\omega_i)+(\rho_n^{\varepsilon}F_\varepsilon'(\Phi),\omega_i).$$

In the last equation we use the fact that $\mathbf{p}\longmapsto\Gamma\boldsymbol{\zeta}$ is linear continuous according to $(\mathbf{H}_3)$. In the other hand, we have the equation $\Lambda(\mathbf{v}_n^{\varepsilon},\psi_n^{\varepsilon})=(\mathbf{u}_n^{\varepsilon},\phi_n^{\varepsilon})$, which mean $(\mathbf{u}_n^{\varepsilon},\phi_n^{\varepsilon})$ solves

$$\begin{aligned}(\rho_n^{\varepsilon}\partial_t\mathbf{u}_n^{\varepsilon},\mathbf{v}_i)+(\rho_n^{\varepsilon}(\mathbf{v}_n^{\varepsilon}\cdot\nabla)\mathbf{u}_n^{\varepsilon},\mathbf{v}_i)+(\nu(\psi_n^{\varepsilon})\mathbb{D}\mathbf{u}_n^{\varepsilon},\nabla\mathbf{v}_i)\\ =(\rho_n^{\varepsilon}\mu_n^{\varepsilon}\nabla\psi_n^{\varepsilon},\mathbf{v}_i)-(\rho_n^{\varepsilon}\nabla(F_\varepsilon(\phi_n^{\varepsilon})),\mathbf{v}_i),\end{aligned}$$

$$(\rho_n^{\varepsilon}\partial_t\phi_n^{\varepsilon},\omega_i)+(\rho_n^{\varepsilon}\mathbf{u}_n^{\varepsilon}\cdot\nabla\psi_n^{\varepsilon},\omega_i)+(\nabla\mu_n^{\varepsilon},\nabla\omega_i)=0,$$

$$(\rho_n^{\varepsilon}\mu_n^{\varepsilon},\omega_i)=(\Gamma\boldsymbol{\xi}(\nabla\phi_n^{\varepsilon}),\nabla\omega_i)+(\rho_n^{\varepsilon}F_\varepsilon'(\phi_n^{\varepsilon}),\omega_i).$$

For all $i = 1, \dots, n$. By uniqueness, it follows that $(U, \Phi, \Upsilon) = (\mathbf{u}_n^\varepsilon, \phi_n^\varepsilon, \mu_n^\varepsilon)$. Thus, every subsequence of $\Lambda(\mathbf{v}_n^{\varepsilon,m}, \psi_n^{\varepsilon,m})$ possesses a subsequence whose limit coincide with $\Lambda(\mathbf{v}_n^\varepsilon, \psi_n^\varepsilon)$, So that the sequence $\Lambda(\mathbf{v}_n^{\varepsilon,m}, \psi_n^{\varepsilon,m})$ converge strongly in $\mathcal{C}^1([0, \widetilde{T}], \mathbf{V}_n \times H_n)$ and its limit is exactly $\Lambda(\mathbf{v}_n^\varepsilon, \psi_n^\varepsilon)$. We deduce that the map Λ is continuous. By the Schauder fixed point theorem, we conclude that, for any $n \in \mathbb{N}$, the map Λ has a fixed point $(\mathbf{u}_n^\varepsilon, \phi_n^\varepsilon)$ on $\mathcal{C}^1([0, \widetilde{T}], \mathbf{V}_n \times H_n)$, wish solves the system (5.37)-(5.40) on $[0, \widetilde{T}]$.

Now we show that the solution is defined on the whole interval $[0, T]$ for any $T > 0$ fixed, instead of $\widetilde{T}$. □

Proposition 2. *Given the initial data $(\rho_{0n}, \mathbf{u}_{0n}, \phi_{0n}, \mu_{0n})$ and let $(\rho_n^\varepsilon, \mathbf{u}_n^\varepsilon, \phi_n^\varepsilon, \mu_n^\varepsilon)$ denote a solution of (5.37)-(5.40) defined in $[0, T_0)$. There is a constant K_0, depending on $(\rho_*, \rho^*, \|\mathbf{u}_0\|_{L^2(\Omega)}, \|\phi_0\|_{H^1(\Omega)})$, but independent of T_0 , such that*

$$\|\mathbf{u}_n^\varepsilon\|_{\mathcal{C}([0,T_0];L^2(\Omega))} + \|\phi_n^\varepsilon\|_{\mathcal{C}([0,T_0];H^1(\Omega))} \leq K_0^2. \tag{5.76}$$

Proof. Multiplying (5.38) by α_i^ε and summing over i we find

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{2}\rho_n^\varepsilon |\mathbf{u}_n^\varepsilon|^2 \mathrm{d}x + \int_\Omega \nu(\phi_n^\varepsilon)|\mathbb{D}(\mathbf{u}_n^\varepsilon)|^2 \mathrm{d}x = \int_\Omega \rho_n^\varepsilon \mu_n^\varepsilon \mathbf{u}_n^\varepsilon \cdot \nabla \phi_n^\varepsilon \mathrm{d}x \\ - \int_\Omega \rho_n^\varepsilon \mathbf{u}_n^\varepsilon \cdot \nabla F_\varepsilon(\phi_n^\varepsilon)\mathrm{d}x. \end{aligned} \tag{5.77}$$

Now, we multiply (5.39) by γ_i^ε and (5.40) by $\frac{\mathrm{d}}{\mathrm{d}t}\beta_i^\varepsilon$, respectively, and summing over i, we get

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left[\frac{1}{2}\Gamma^2(\nabla\phi_n^\varepsilon) + \rho_n^\varepsilon F_\varepsilon(\phi_n^\varepsilon)\right]\mathrm{d}x + \int_\Omega \rho_n^\varepsilon \mathbf{u}_n^\varepsilon \cdot \nabla\phi_n^\varepsilon \mu_n^\varepsilon \mathrm{d}x \quad + \int_\Omega D(\phi_n^\varepsilon)|\nabla\mu_n^\varepsilon|^2 \mathrm{d}x \\ = \int_\Omega \partial_t \rho_n^\varepsilon F_\varepsilon(\phi_n^\varepsilon)\mathrm{d}x. \end{aligned} \tag{5.78}$$

By summing the previous equation (5.77) and (5.78), we obtain

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{2}\rho_n^\varepsilon \left|\mathbf{u}_n^\varepsilon\right|^2 + \frac{1}{2}\Gamma^2\left(\nabla\phi_n^\varepsilon\right) + \rho_n^\varepsilon F_\varepsilon\left(\phi_n^\varepsilon\right)\mathrm{d}x \\ + \int_\Omega \nu\left(\phi_n^\varepsilon\right)\left|\mathbb{D}\mathbf{u}_n^\varepsilon\right|^2 + D(\phi_n^\varepsilon)\left|\nabla\mu_n^\varepsilon\right|^2 \mathrm{d}x = 0. \end{aligned} \tag{5.79}$$

Integrating in time over $[0,t]$ where $0 < t < T_0$, we deduce that

$$\begin{aligned}
&\int_\Omega \frac{1}{2}\rho_n^\varepsilon(t)\left|\mathbf{u}_n^\varepsilon(t)\right|^2 + \frac{1}{2}\Gamma^2\left(\nabla\phi_n^\varepsilon(t)\right) + \rho_n^\varepsilon(t)F_\varepsilon\left(\phi_n^\varepsilon(t)\right)\mathrm{d}x \\
&\quad + \int_0^t\int_\Omega \nu\left(\phi_n^\varepsilon(\tau)\right)\left|\mathbb{D}\mathbf{u}_n^\varepsilon(\tau)\right|^2\mathrm{d}x\mathrm{d}\tau + \int_0^t\int_\Omega D(\phi_n^\varepsilon(\tau))\left|\nabla\mu_n^\varepsilon(\tau)\right|^2\mathrm{d}x\mathrm{d}\tau \qquad (5.80)\\
&\quad = \int_\Omega \frac{1}{2}\rho_{0n}\left|\mathbf{u}_{0n}\right|^2 + \frac{1}{2}\Gamma^2\left(\nabla\phi_{0n}\right) + \rho_{0n}F_\varepsilon\left(\phi_{0n}\right)\mathrm{d}x.
\end{aligned}$$

Using the properties of the projector operator P_n^1 and P_n^2, we find

$$\begin{aligned}
&\int_\Omega \frac{1}{2}\rho_{0n}\left|\mathbf{u}_{0n}\right|^2 + \frac{1}{2}\Gamma^2\left(\nabla\phi_{0n}\right) + \rho_{0n}F_\varepsilon\left(\phi_{0n}\right)\mathrm{d}x \\
&\qquad \le \frac{\rho^*}{2}\|\mathbf{u}_0\|_{L^2(\Omega)}^2 + \frac{R}{2}\|\phi_0\|_{H^1(\Omega)}^2 + K(\varepsilon)\rho^*\left(1 + \|\phi_0\|_{H^1(\Omega)}^4\right),
\end{aligned}$$

where the constant $K(\varepsilon)$ is independent of n. Since $F_\varepsilon(s) \ge 0$, we obtain

$$\begin{aligned}
\frac{\rho_*}{2}\|\mathbf{u}_n^\varepsilon(t)\|_{L^2(\Omega)}^2 + \frac{r}{2}\|\nabla\phi_n^\varepsilon(t)\|_{L^2(\Omega)}^2 \le \frac{\rho^*}{2}\|\mathbf{u}_0\|_{L^2(\Omega)}^2 + \frac{R}{2}\|\phi_0\|_{H^1(\Omega)}^2 \\
+ K(\varepsilon)\rho^*\left(1 + \|\phi_0\|_{H^1(\Omega)}^4\right).
\end{aligned}$$

Therefore, there exists a positive constant $K_0 = K_0\left(\varepsilon, \rho_*, \rho^*, \mathbf{u}_0, \phi_0, r, R\right)$ such that

$$\sup_{[0,T_0]}\|\mathbf{u}_n^\varepsilon(t)\|_{L^2(\Omega)} + \sup_{[0,T_0]}\|\phi_n^\varepsilon(t)\|_{H^1(\Omega)} \le K_0^2.$$

□

The proposition 2 shows that if a solution exists on the time interval $[0, T_0)$, then this solution cannot explode near T_0. Consequently, we conclude that there exists a global existence of the Galerkin approximate sequence that solves the system (5.37)-(5.40).

5.6 PROOF OF THE GLOBAL EXISTENCE THEOREM 1

In this section we prove Theorem 1: the proof is split into two parts. Firstly, we derive estimates on the solutions of the Galerkin approximate problem (5.37)-(5.40), independently of n. Secondly, we pass to the limit as $n \to \infty$ and recover weak solutions of the regularized problem. Thirdly, with the same way we obtain

estimates on solutions of the regularized problem (5.24)-(5.27) independently of ε. We pass to the limit as $\varepsilon \to 0^+$ and recover weak solutions of the problem (5.1)-(5.4).

Starting from (5.80) we obtain

$$E^\varepsilon(\rho_n^\varepsilon(t), \mathbf{u}_n^\varepsilon(t), \phi_n^\varepsilon(t)) + \int_0^t \int_\Omega \nu\left(\phi_n^\varepsilon(\tau)\right) |\mathbb{D}\mathbf{u}_n^\varepsilon(\tau)|^2 + D(\phi_n^\varepsilon(\tau)) \left|\nabla \mu_n^\varepsilon(\tau)\right|^2 \mathrm{d}x\mathrm{d}\tau = E^\varepsilon(\rho_{0n}, \mathbf{u}_{0n}, \phi_{0n}). \tag{5.81}$$

From (5.31) it follows that $E^\varepsilon(\rho_{0n}, \mathbf{u}_{0n}, \phi_{0n})$ converge to $E^\varepsilon(\rho_0, \mathbf{u}_0, \phi_0)$ as $n \to \infty$. where

$$E^\varepsilon(\rho_0, \mathbf{u}_0, \phi_0) = \int_\Omega \frac{1}{2}\rho_0 |u_0|^2 + \frac{1}{2}\Gamma^2(\nabla\phi_0) + \rho_0 F_\varepsilon(\phi_0)\mathrm{d}x := E_0^\varepsilon.$$

Since $F_\varepsilon \geq 0$, we have for n sufficiently large

$$\|\mathbf{u}_n^\varepsilon(t)\|_{L^2(\Omega)}^2 + \|\nabla\phi_n^\varepsilon(t)\|_{L^2(\Omega)}^2 \leq \max\left\{\frac{2}{r}, \frac{2}{\rho_*}\right\} E^\varepsilon(\rho_0, \mathbf{u}_0, \phi_0). \tag{5.82}$$

Consequently, there exists a constant $C = C(\varepsilon, \rho_*, \nu_*, D_*, r)$ such that

$$\|\mathbf{u}_n^\varepsilon\|_{L^\infty(0,T;\mathbf{H})} \leq C\sqrt{E_0^\varepsilon}, \tag{5.83}$$

$$\|\mathbf{u}_n^\varepsilon\|_{L^2(0,T;\mathbf{V})} \leq C\sqrt{E_0^\varepsilon}, \tag{5.84}$$

$$\|\nabla\phi_n^\varepsilon\|_{L^\infty(0,T;L^2(\Omega))} \leq C\sqrt{E_0^\varepsilon}, \tag{5.85}$$

$$\|\nabla\mu_n^\varepsilon\|_{(0,T;L^2(\Omega))} \leq C\sqrt{E_0^\varepsilon}. \tag{5.86}$$

Similar estimates to those in the isotropic case can be obtained [Giorgini and Temam, 2020]

$$\|\rho_n^\varepsilon\|_{L^\infty(0,T;H^{-1}(\Omega))} \leq C, \tag{5.87}$$

$$\|\phi_n^\varepsilon\|_{L^\infty(0,T;H^1(\Omega))} \leq C, \tag{5.88}$$

$$\|\mu_n^\varepsilon\|_{L^2(0,T;H^1(\Omega))} \leq C, \tag{5.89}$$

$$\|\phi_n^\varepsilon\|_{B^{\frac{1}{4}}_{\infty,\infty}(0,T;L^2(\Omega))} \leq C. \tag{5.90}$$

For some positive constant $C := C(\varepsilon, T)$ independent of n.

To estimate $\|\mathbf{u}_n^\varepsilon\|_{B^{\frac{1}{4}}_{2,\infty}(0,T;\mathbf{H})}$, let fix h such that $0 < h < T$. For $0 \leq t \leq T - h$ we test (5.38) at time τ by $\mathbf{u}_n^\varepsilon(t+h) - \mathbf{u}_n^\varepsilon(t)$ and (5.37) at time τ by $\mathbf{u}_n^\varepsilon(t) \cdot (\mathbf{u}_n^\varepsilon(t+$

$h) - \mathbf{u}_n^\varepsilon(t))$. After integration with respect to τ from t to $t+h$ and some obvious manipulations we arrive at

$$\begin{aligned}
\int_\Omega \rho_n^\varepsilon(t+h)\left|\mathbf{u}_n^\varepsilon(t+h)-\mathbf{u}_n^\varepsilon(t)\right|^2 \mathrm{d}x = \\
&\underbrace{\int_\Omega -\left(\rho_n^\varepsilon(t+h)-\rho_n^\varepsilon(t)\right)\mathbf{u}_n^\varepsilon(t)\cdot\left(\mathbf{u}_n^\varepsilon(t+h)-\mathbf{u}_n^\varepsilon(t)\right)\mathrm{d}x}_{I_1(t)} \\
&+\underbrace{\int_t^{t+h}\int_\Omega -\operatorname{div}\left(\rho_n^\varepsilon(\tau)\mathbf{u}_n^\varepsilon(\tau)\otimes\mathbf{u}_n^\varepsilon(\tau)\right)\cdot\left(\mathbf{u}_n^\varepsilon(t+h)-\mathbf{u}_n^\varepsilon(t)\right)\mathrm{d}x\mathrm{d}\tau}_{I_2(t)} \\
&+\underbrace{\int_t^{t+h}\int_\Omega -\nu\left(\phi_n^\varepsilon(\tau)\right)\mathbb{D}\mathbf{u}_n^\varepsilon(\tau):\nabla\left(\mathbf{u}_n^\varepsilon(t+h)-\mathbf{u}_n^\varepsilon(t)\right)\mathrm{d}x\mathrm{d}\tau}_{I_3(t)} \\
&+\underbrace{\int_t^{t+h}\int_\Omega \rho_n^\varepsilon(\tau)\mu_n^\varepsilon(\tau)\nabla\phi_n^\varepsilon(\tau)\cdot\left(\mathbf{u}_n^\varepsilon(t+h)-\mathbf{u}_n^\varepsilon(t)\right)\mathrm{d}x\mathrm{d}\tau}_{I_4(t)} \\
&+\underbrace{\int_t^{t+h}\int_\Omega -\rho_n^\varepsilon(\tau)F_\varepsilon'\left(\phi_n^\varepsilon(\tau)\right)\nabla\phi_n^\varepsilon(\tau)\cdot\left(\mathbf{u}_n^\varepsilon(t+h)-\mathbf{u}_n^\varepsilon(t)\right)\mathrm{d}x\mathrm{d}\tau}_{I_5(t)}.
\end{aligned} \tag{5.91}$$

In the isotropic case ($\Gamma(\nabla\phi)=|\nabla\phi|$), we can control $\|\phi_n\|_{H^2(\Omega)}$ independently of n. However, in the anisotropic case, this argument is not applicable. Alternatively, to estimate $\|\mathbf{u}_n\|_{B^{\frac{1}{4}}_{2,\infty}(0,T;\mathbf{H})}$, it follows along the same lines of Giorgini and Temam [2020] (page 210) that $\int_0^{T-h}|I_k(t)|\mathrm{d}t \le Ch^{\frac{1}{2}}$ for $k=1,2,3$ and 4, with C is a constant independent of n. Thus, it is sufficient to control $I_5(t)$

$$I_5(t)=\int_t^{t+h}\int_\Omega -\rho_n^\varepsilon(\tau)F_\varepsilon'\left(\phi_n(\tau)\right)\nabla\phi_n^\varepsilon(\tau)\cdot\left(\mathbf{u}_n^\varepsilon(t+h)-\mathbf{u}_n^\varepsilon(t)\right)\mathrm{d}x\mathrm{d}\tau.$$

$$\begin{aligned}
|I_5(t)| &\le \rho^*\int_t^{t+h}\left\|F_\varepsilon'\left(\phi_n^\varepsilon(\tau)\right)\right\|_{L^6(\Omega)}\left\|\nabla\phi_n^\varepsilon(\tau)\right\|_{L^2(\Omega)}\mathrm{d}\tau\left\|\mathbf{u}_n^\varepsilon(t+h)-\mathbf{u}_n^\varepsilon(t)\right\|_{L^3(\Omega)} \\
&\le C\int_t^{t+h}\left\|F_\varepsilon'\left(\phi_n^\varepsilon(\tau)\right)\right\|_{L^6(\Omega)}\mathrm{d}\tau\left(\left\|\nabla\mathbf{u}_n^\varepsilon(t+h)\right\|_{L^2(\Omega)}^{\frac{1}{2}}+\left\|\nabla\mathbf{u}_n^\varepsilon(t)\right\|_{L^2(\Omega)}^{\frac{1}{2}}\right).
\end{aligned}$$

Integrating from 0 to $T-h$, we find

$$\int_0^{T-h} |I_5(t)| \, \mathrm{d}t \leq Ch^{\frac{3}{4}} \int_0^T \|F_\varepsilon'(\phi_n^\varepsilon(\tau))\|_{L^6(\Omega)} \, \mathrm{d}\tau.$$

We have

$$\begin{aligned}\|F_\varepsilon'(\phi_n^\varepsilon(\tau))\|_{L^6(\Omega)}^6 &= \int_{|\phi_n^\varepsilon|\leq 1-\varepsilon} |F_\varepsilon'(\phi_n^\varepsilon(\tau))|^6 \mathrm{d}x + \int_{|\phi_n^\varepsilon|\geq 1-\varepsilon} |F_\varepsilon'(\phi_n^\varepsilon(\tau))|^6 \mathrm{d}x \\ &\leq \left(\lambda_2(1-\varepsilon) + \frac{\lambda_1}{2}\log(1+\varepsilon/2) + |\log(\varepsilon/2)|\right)^6 |\Omega| + \int_{|\phi_n^\varepsilon|\geq 1-\varepsilon} |F_\varepsilon'(\phi_n^\varepsilon(\tau))|^6 \mathrm{d}x\end{aligned}$$

On the domain $\{s \in \mathbb{R}\,;\, |s| \geq 1-\varepsilon\}$, the function F_ε' is polynomial of degree one. Since $\|\phi_n^\varepsilon\|_{H^1(\Omega)} \leq C(\varepsilon)$ and the fact that $H^1(\Omega) \hookrightarrow L^6(\Omega)$ (for $d = 2, 3$) , we get

$$\int_0^{T-h} |I_5(t)| \, \mathrm{d}t \leq C(\varepsilon)h^{\frac{3}{4}}.$$

Then, we deduce that

$$\|\mathbf{u}_n^\varepsilon\|_{B^{\frac{1}{4}}_{2,\infty}(0,T;\mathbf{H})} \leq C(\varepsilon, T). \tag{5.92}$$

With the uniform estimates in hand (5.87)-(5.90)-(5.92), we can use a compactness argument to prove that a subsequence of the approximate sequence tends to some function $(\rho^\varepsilon, \mathbf{u}^\varepsilon, \phi^\varepsilon, \mu^\varepsilon)$ which satisfies the system (5.24)-(5.27) in the sense of distribution. Since the proof is very similar to Giorgini and Temam [2020], here, we omit the details for brevity. The only difference with Giorgini and Temam [2020], is taking the limit of the quantity $\Gamma\boldsymbol{\zeta}(\nabla\phi_n^\varepsilon) \otimes \nabla\phi_n^\varepsilon$. However, according to assumption $(\mathbf{H}_2)$, the map $\mathbf{p} \mapsto \Gamma\boldsymbol{\zeta}(\mathbf{p})$ is linear, and thus continuous. On the other hand, one can show that $\phi_n^\varepsilon \to \phi^\varepsilon$ strongly in $L^4(0,T;H^1(\Omega))$, which implies that

$$\Gamma\boldsymbol{\zeta}(\nabla\phi_n^\varepsilon) \otimes \nabla\phi_n^\varepsilon \to \Gamma\boldsymbol{\zeta}(\nabla\phi^\varepsilon) \otimes \nabla\phi^\varepsilon \text{ strongly in } L^2(0,T;L^2(\Omega)). \tag{5.93}$$

Furthermore, the equation (5.27) holds almost everywhere in $(0,T) \times \Omega$.

Proposition 3. *There exists a constant $C(T) > 0$ such that, for all $\varepsilon \in (0, 1 - \sqrt{1-\lambda_2/\lambda_1})$, it holds*

$$\|\rho^\varepsilon\|_{L^\infty(0,T;H^{-1}(\Omega))} \leq C(T), \tag{5.94}$$

$$\|\phi^\varepsilon\|_{L^\infty(0,T;H^1(\Omega))} \leq C(T), \tag{5.95}$$

$$\|\mu^\varepsilon\|_{L^2(0,T;H^1(\Omega))} \leq C(T), \tag{5.96}$$

$$\|\phi^\varepsilon\|_{B^{\frac{1}{4}}_{\infty,\infty}(0,T;L^2(\Omega))} \leq C(T), \tag{5.97}$$

$$\|\mathbf{u}^\varepsilon\|_{B^{\frac{1}{4}}_{2,\infty}(0,T;\mathbf{H})} \leq C(T). \tag{5.98}$$

Proof. First of all, we have the density bounds

$$\rho_* \leq \rho_\varepsilon(x,t) \leq \rho^* \quad \text{ a.e. in } \Omega \times (0,T). \tag{5.99}$$

Using similar lines of the proof 5.5 to the regularized problem 5.24–5.27 we find

$$\begin{aligned}
&\int_\Omega \frac{1}{2}\rho^\varepsilon(t)\left|\mathbf{u}^\varepsilon(t)\right|^2 + \frac{1}{2}\Gamma^2\left(\nabla\phi^\varepsilon(t)\right) + \rho^\varepsilon(t)F_\varepsilon\left(\phi^\varepsilon(t)\right)\mathrm{d}x \\
&\quad + \int_0^t\int_\Omega \nu\left(\phi^\varepsilon(\tau)\right)\left|\mathbb{D}\mathbf{u}^\varepsilon(\tau)\right|^2\mathrm{d}x\mathrm{d}\tau + \int_0^t\int_\Omega D(\phi^\varepsilon(\tau))\left|\nabla\mu^\varepsilon(\tau)\right|^2\mathrm{d}x\mathrm{d}\tau \\
&\quad = \int_\Omega \frac{1}{2}\rho_0\left|\mathbf{u}_0\right|^2 + \frac{1}{2}\Gamma^2\left(\nabla\phi_0\right) + \rho_0 F_\varepsilon\left(\phi_0\right)\mathrm{d}x := E_0^\varepsilon.
\end{aligned} \tag{5.100}$$

Since $\|\phi_0\|_{L^\infty} \leq 1$, and according to (5.23), we have

$$E_0^\varepsilon \leq \int_\Omega \frac{1}{2}\rho_0|u_0|^2 + \frac{1}{2}\Gamma^2(\nabla\phi_0) + \rho_0 F(\phi_0)\mathrm{d}x := E_0, \tag{5.101}$$

and the inequalities (5.94)–(5.97) follows easily. For the last inequality (5.98), we

proceed as in (5.91), we have

$$\begin{aligned}\int_\Omega \rho^\varepsilon(t+h)\left|\mathbf{u}^\varepsilon(t+h)-\mathbf{u}^\varepsilon(t)\right|^2\mathrm{d}x = \\ \underbrace{\int_\Omega -\left(\rho^\varepsilon(t+h)-\rho^\varepsilon(t)\right)\mathbf{u}^\varepsilon(t)\cdot\left(\mathbf{u}^\varepsilon(t+h)-\mathbf{u}^\varepsilon(t)\right)\mathrm{d}x}_{J_1(t)} \\ + \underbrace{\int_t^{t+h}\int_\Omega -\operatorname{div}\left(\rho^\varepsilon(\tau)\mathbf{u}^\varepsilon(\tau)\otimes\mathbf{u}^\varepsilon(\tau)\right)\cdot\left(\mathbf{u}^\varepsilon(t+h)-\mathbf{u}^\varepsilon(t)\right)\mathrm{d}x\mathrm{d}\tau}_{J_2(t)} \\ + \underbrace{\int_t^{t+h}\int_\Omega -\nu\left(\phi^\varepsilon(\tau)\right)\mathbb{D}\mathbf{u}^\varepsilon(\tau):\nabla\left(\mathbf{u}^\varepsilon(t+h)-\mathbf{u}^\varepsilon(t)\right)\mathrm{d}x\mathrm{d}\tau}_{J_3(t)} \\ + \underbrace{\int_t^{t+h}\int_\Omega \rho^\varepsilon(\tau)\mu^\varepsilon(\tau)\nabla\phi^\varepsilon(\tau)\cdot\left(\mathbf{u}^\varepsilon(t+h)-\mathbf{u}^\varepsilon(t)\right)\mathrm{d}x\mathrm{d}\tau}_{J_4(t)} \\ + \underbrace{\int_t^{t+h}\int_\Omega -\rho^\varepsilon(\tau)F_\varepsilon'\left(\phi^\varepsilon(\tau)\right)\nabla\phi^\varepsilon(\tau)\cdot\left(\mathbf{u}^\varepsilon(t+h)-\mathbf{u}^\varepsilon(t)\right)\mathrm{d}x\mathrm{d}\tau}_{J_5(t)}.\end{aligned} \tag{5.102}$$

Same here, $\int_0^{T-h}|J_k(t)|\mathrm{d}t \le Ch^{\frac{1}{2}}$ for $k=1,2,3$ and 4, with C is a constant independent of ε. Thus, it is sufficient to control $J_5(t)$ by bounding $\|F_\varepsilon'(\phi^\varepsilon)\|_{L^2(0,T;L^6(\Omega))}$ independently of ε. To do, let show that

$$\|G_\varepsilon'(\phi^\varepsilon)\|_{L^2(0,T;L^6(\Omega))} \le C.$$

where C is a constant independent of ε. The argument is inspired from Abels [2009], we define for all $k>1$

$$\phi_k^\epsilon = h_k\circ\phi^\varepsilon, \quad h_k(s) = \begin{cases} 1-\frac{1}{k} & s>1-\frac{1}{k}, \\ s & -1+\frac{1}{k}\le s\le 1-\frac{1}{k}, \\ -1+\frac{1}{k} & s<-1+\frac{1}{k}. \end{cases}$$

The chain rule holds $\nabla\phi_k^\varepsilon = \nabla\phi^\varepsilon\chi_{\left[-1+\frac{1}{k},1-\frac{1}{k}\right]}(\phi^\varepsilon)$.

Now, multiplying (5.27) by $|G'_\varepsilon(\phi_k^\varepsilon)|^4 G'_\varepsilon(\phi_k^\varepsilon)$ and integrating over Ω, we find

$$\int_\Omega |G'_\varepsilon(\phi_k^\varepsilon)|^4 G''_\varepsilon(\phi_k^\varepsilon)\,\Gamma\boldsymbol{\zeta}(\nabla\phi^\varepsilon)\cdot\nabla\phi_k^\varepsilon \mathrm{d}x + \int_\Omega \rho^\varepsilon |G'_\varepsilon(\phi_k^\varepsilon)|^4 G'_\varepsilon(\phi_k^\varepsilon) G'_\varepsilon(\phi^\varepsilon)dx$$
$$= \int_\Omega (\rho^\varepsilon\mu^\varepsilon + \lambda_1\rho^\varepsilon\phi^\varepsilon)|G'_\varepsilon(\phi_k^\varepsilon)|^4 G'_\varepsilon(\phi_k^\varepsilon)\,dx.$$

According to the assumption $\mathbf{H}_3$ and the fact that G_ε is strictly convex, the first term on the left-hand side is non-negative. We also have that $G'_\varepsilon(\phi_k^\varepsilon)^2 \leq G'_\varepsilon(\phi^\varepsilon)G'_\varepsilon(\phi_k^\varepsilon)$ almost everywhere. Thus, by Young's inequality, we obtain

$$\|G'_\varepsilon(\phi_k^\varepsilon)\|^6_{L^6(\Omega)} \leq C\,\|\rho^\varepsilon\mu^\varepsilon + \lambda_1\rho^\varepsilon\phi^\varepsilon\|^6_{L^6(\Omega)},$$

From (5.99), (5.95) and (5.96), we get $\rho^\varepsilon\mu^\varepsilon + \lambda_1\rho^\varepsilon\phi^\varepsilon \in L^2(0,T;L^6(\Omega))$. Then, there exist a constant $C := C(\rho_*, \rho^*, E_0, \lambda_1)$ independent of ε and k such that

$$\|G'_\varepsilon(\phi_k^\varepsilon)\|_{L^2(0,T;L^6(\Omega))} \leq C$$

By applying Fatou's lemma, we have

$$\|G'_\varepsilon(\phi^\varepsilon)\|_{L^2(0,T;L^6(\Omega))} \leq C$$

Since $F'(\phi^\varepsilon) = -\lambda_1\phi^\varepsilon + G'_\varepsilon(\phi^\varepsilon)$, we deduce that $\|F'_\varepsilon(\phi^\varepsilon)\|_{L^2(0,T;L^6(\Omega))}$ bounded independently of ε, i.e

$$\|F'_\varepsilon(\phi^\varepsilon)\|_{L^2(0,T;L^6(\Omega))} \leq C.$$

□

By recalling the proposition 3, the compact embedding, and same as (5.93), we have

$$\Gamma\boldsymbol{\zeta}(\nabla\phi^\varepsilon)\otimes\nabla\phi^\varepsilon \to \Gamma\boldsymbol{\zeta}(\nabla\phi)\otimes\nabla\phi \text{ strongly in } L^2(0,T;L^2(\Omega)),$$

we can infer that there exist some functions $(\rho, \mathbf{u}, \phi, \mu)$ with

$$\rho \in \mathcal{C}([0,T];L^2(\Omega)) \cap L^\infty(\Omega\times(0,T)) \cap W^{1,\infty}\left(0,T;H^{-1}(\Omega)\right), \tag{5.103}$$
$$\mathbf{u} \in L^2(0,T;\mathbf{V}) \cap B^{\frac{1}{4}}_{2,\infty}(0,T;\mathbf{H}), \tag{5.104}$$
$$\phi \in L^2\left(0,T;H^1(\Omega)\right) \cap B^{\frac{1}{4}}_{\infty,\infty}\left(0,T;L^2(\Omega)\right), \tag{5.105}$$
$$\mu \in L^2\left(0,T;H^1(\Omega)\right). \tag{5.106}$$

And we thus complete the proof of Theorem 1.

5.7 CONCLUSION AND PERSPECTIVE

In this chapter, we established the global existence of weak solutions for the incompressible anisotropic Cahn–Hilliard–Navier–Stokes (CHNS) system in both two and three spatial dimensions. By incorporating anisotropic surface energy—which extends the standard isotropic energy by using a general function $\Gamma(\nabla\phi)$—we advanced beyond prior CHNS models that primarily assumed isotropy. Our proof uses a Galerkin approximation scheme, supplemented by novel applications of Bihari's inequality and a fixed-point argument, ensuring global-in-time control of the approximate solutions and allowing passage to the limit . This approach overcomes key challenges in managing the higher-order nonlinearities introduced by anisotropy. The result broadens the mathematical foundations for modeling two-phase flows with complex interfacial energies, offering a rigorous existence theory for anisotropic CHNS models that better reflect physical scenarios with directional-dependent interfacial effects.

This work opens several interesting directions for future research. One of the principal challenges is the analysis of uniqueness and the potential existence of strong solutions in the anisotropic setting. The complexity introduced by anisotropic surface energies remains a rich area for further mathematical investigation.

In the present study, we considered the free energy functional to be of the form $\int_\Omega \frac{1}{2}\Gamma^2(\nabla\phi)$, which corresponds to the case $a = 0$ (see Equation (3.162) in Section 3.4.3). As discussed in Section 3.4, this formulation follows the model proposed by Anderson et al. [2000]. An alternative approach, inspired by the formulation of Guo and Lin [2015], is to take the free energy functional as $\int_\Omega \frac{1}{2}\rho\Gamma^2(\nabla\phi)$, which corresponds to the case $a = 1$ (see Equation (3.154) in Section 3.4.3). Investigating this variant would provide insight into the interplay between density and interface energy, and it could lead to different mathematical behaviors and analytical challenges. These perspectives underline the versatility of the CHNS framework and encourage further exploration of its thermodynamically consistent generalizations.

CHAPTER

TWO VELOCITY MODEL PROBLEM 6

6.1 INTRODUCTION

An ideal multi-fluid is a mixture of two or more phases of matter with dissipative effects taken to be zero, and with negligible dynamic and thermodynamic effects between the phases. Thus, dissipative, frictional and drag and virtual mass forces are not taken into account. The dynamics of the mixture is called a multi-phase flow, and this dynamics depends on the nature of the phases present and their interfacial structure. The most common class of multi-phase flows are the two-phase flows, and these include gas-liquid flow, gas-solid flow, liquid-liquid flow and liquid-solid flow. Our study is focused on the first three: we will present some models that describe dispersed flows, i.e., bubbles in liquid, sprays, ... etc. We note, that one type of model that describes flows of these type of mixtures are called Euler-Euler models [Ishii and Hibiki, 2010].

Let us briefly recall the so-called Lagrangian variable or material description [Morrison, 1998a, Morrison et al., 2020, Morrison, 2006, Drui et al., 2019]. In this description, we follow the trajectories of mixture "particles", i.e. infinitesimal elements or parcels, of each constituent, labeled by their initial position $\mathbf{a}$. For a two phase mixture we have two possible trajectories: $\mathbf{q}_k(\mathbf{a}, t) \in \Omega$ for $k = 1, 2$, which give the position of particle "k" labeled by $\mathbf{a} \in \Omega$ at time $t \in \mathbb{R}$. Here $\Omega \subset \mathbb{R}^3$ denotes the physical domain occupied by the mixture. Thus, the configuration space is the space of diffeomorphisms, smooth coordinated changes $\mathbf{a} \mapsto \mathbf{q}_k$, of the space $\Omega \times \Omega$.

Its cotangent space then has the two momenta $\boldsymbol{\pi}_k$, and the cotangent bundle with coordinates $(\mathbf{q}_1, \mathbf{q}_2, \boldsymbol{\pi}_1, \boldsymbol{\pi}_2)$ is the phase space of the mixture.

In the Hamiltonian framework of the Lagrangian description of fluids, we attach attributes to a fluid element – here we will refer to fluid elements as particles while keeping in mind that we are considering a continuum theory. For example, in single-phase fluid we would attach a density $\rho_0(\mathbf{a})$ to a fluid element akin to identifying a mass m_i to the ith particle in a *genuine* particle description; here the continuum label $\mathbf{a}$ is akin to the index i. However, for a multi-phase flow, the situation is more complicated. For particles of each phase we attach a mass density $\hat{\rho}_k(\mathbf{a}, t)$, an entropy density $\hat{\sigma}_k(\mathbf{a}, t)$, and a momentum density $\hat{\mathbf{M}}_k(\mathbf{a}, t)$. In the following we will use hat notations for Lagrangian quantities, with the exception of $\mathbf{q}_k$ and its derivatives, to distinguish Lagrangian from Eulerian quantities (defined below). Also, we use

$$\mathbf{q}_k(\mathbf{a}, t) = (q_k^1, q_k^2, q_k^3) \quad \text{and} \quad \mathbf{q}_k(\mathbf{a}, 0) = \mathbf{a} = (a^1, a^2, a^3)\,, \tag{6.1}$$

where in index notation we have q_k^i and a_k^i, for $i = 1, 2, 3$, and we have decided to label the particles of each phase by their initial positions in Ω.

The Lagrangian (and Eulerian) description of two-phase flows has some similarity to that of the two fluid description of plasmas [D'Avignon et al., 2016], which uses one fluid for electrons and a second for ions. However, there is an important difference: both electrons and ions in the plasma description are assumed to completely fill infinitesimal volumes, while in two-phase flow the constituents of the individual phases can each partially fill an infinitesimal volume. To account for this the volume fraction $\hat{\alpha}_k(t, \mathbf{a})$ is introduced – it accounts for the amount of each phase contained in an infinitesimal volume element.

Instead of following particle trajectories, in the Eulerian description we examine the flow at an observation point $\mathbf{r} = (r^1, r^2, r^3) \in \Omega$ at any time t. For a single phase fluid, we would have the Eulerian velocity field $\mathbf{u}(\mathbf{r}, t)$, the mass density $\rho(\mathbf{r}, t)$ and the specific entropy $s(\mathbf{r}, t)$, which might be governed by the Navier-Stokes equations. For a two-phase flow, we have in general two of each, i.e., $\mathbf{u}_k(\mathbf{r}, t)$, $\rho_k(\mathbf{r}, t)$, and $s_k(\mathbf{r}, t)$, for $k = 1, 2$, and we have the Eulerian volume fraction $\alpha_k(\mathbf{r}, t)$. Because an infinitesimal volume is assumed to be filled, by a mixture of both phases, we have

$$\alpha_1(\mathbf{r}, t) + \alpha_2(\mathbf{r}, t) = 1\,. \tag{6.2}$$

Thus, the total mass density is

$$\rho = \alpha_1\rho_1 + \alpha_2\rho_2 =: \tilde{\rho}_1 + \tilde{\rho}_2\,, \tag{6.3}$$

and $\tilde{\rho}_k$ is the actual density of phase k per the volume it occupies.

The Eulerian description observes attributes and velocities of particles that are located at $\mathbf{r}$ at time t. Thus, the Lagrange-Euler map follows from $\mathbf{q}_k(\mathbf{a}, t) = \mathbf{r}$, where it is assumed that the trajectory maps $\mathbf{a} \mapsto \mathbf{q}_k(\mathbf{a}, t)$ are not only smooth but invertible. For an arbitrary function we use the notation

$$\hat{f}_k(\mathbf{a}, t) = f_k(\mathbf{r}, t)\,, \tag{6.4}$$

where the Lagrangian quantity $\hat{f}_k$ on the left is defined upon inserting $\mathbf{r} = \mathbf{q}_k(\mathbf{a}, t)$ into f_k on the right, or the Eulerian quantity on the right is defined upon inserting the inverse $\mathbf{a} = \mathbf{q}_k^{-1}(\mathbf{r}, t)$ into $\hat{f}_k$ on the left. We will further refine the Lagrangian and Eulerian descriptions in subsequent sections.

Until this point we have been very general, but now some simplifications that exist in the literature are made. In particular, the following dichotomy is considered: either $\mathbf{q}_1(\mathbf{a}, t) \neq \mathbf{q}_2(\mathbf{a}, t)$, where the two phases move on different trajectories, or $\mathbf{q}_1(\mathbf{a}, t) = \mathbf{q}_2(\mathbf{a}, t)$, where they are "stuck" and move together. These define two classes of two-phase flows: A first class where $\mathbf{q}_1 \neq \mathbf{q}_2$, implying the respective velocity fields have $\mathbf{u}_1 \neq \mathbf{u}_2$. These models are called Two Velocity models (TVMs) [Ishii and Hibiki, 2010]. The second class of models assumes the particles of phases "1" and "2", initialized $t = 0$ at a same position $\mathbf{a}$, move on the same path. Thus they move with the same velocity field, say $\mathbf{u}$. These models are called One Velocity models [Ishii and Hibiki, 2010] or, as we will call them, Zero Drift Flux Models (zDFMs) after Bansal et al. [2021].

In Table 6.1 we summarize some common notation for flows with two phases:

Symbol	Description $1, 2$	Symbol	Description $1, 2$
$\alpha_{1,2}$:	Volume fraction	$\eta_{1,2}$:	Mass fraction
$\rho_{1,2}$:	Density	$v_{1,2}$:	Specific volume $\left(=\frac{1}{\rho_{1,2}}\right)$
$c_{1,2}$:	Adiabatic speed of sound	$e_{1,2}$:	Specific internal energy
$s_{1,2}$:	Specific entropy	$E_{1,2}$:	Specific total energy
$p_{1,2}$:	Pressure	$H_{1,2}$:	Specific total enthalpy
$\mathbf{u}_{1,2}$:	Velocity	$T_{1,2}$:	Temperature
$\mu_{1,2}$:	Viscosity	$h_{1,2}$:	Specific enthalpy
$\Gamma_{1,2}$:	Grüneisen parameter	$\mathrm{Kn}_{1,2}$:	Knudsen numbers

6.2 TWO-VELOCITY MODEL (TVM)

Consider now in detail both the Lagrangian and Eulerian descriptions of the TVM. At the Eulerian observation position $\mathbf{r} \in \Omega$ at time t, there exists a mixture, a portion of which can be viewed as comprised of a particles of phase "1" and a portion of which is comprised of a particle of phase "2". Note, because $\mathbf{q}_1 \neq \mathbf{q}_2$, the particles arriving at $\mathbf{r}$ at time t come from different initial positions, say $\mathbf{a}_1, \mathbf{a}_2$. Thus we have

$$\mathbf{r} = \mathbf{q}_1(\mathbf{a}_1, t) = \mathbf{q}_2(\mathbf{a}_2, t) \tag{6.5}$$

where $\mathbf{a}_1 \neq \mathbf{a}_2$. This complication was previously explored in the plasma magnetofluid context in [D'Avignon et al., 2016], although as noted above, volume fractions do not appear in the plasma theory. Here, we have the "total volume" formula

$$\hat{\alpha}_1(\mathbf{a}_1, t) + \hat{\alpha}_2(\mathbf{a}_2, t) = 1\,, \tag{6.6}$$

and because $\mathbf{a}_2 = \mathbf{q}_2^{-1}(\mathbf{q}_1(t, \mathbf{a}_1), t)$, we can rewrite (6.6) as

$$\hat{\alpha}_1(\mathbf{a}_1, t) + \hat{\alpha}_2(\mathbf{q}_2^{-1}(\mathbf{q}_1(\mathbf{a}_1, t), t)) = 1\,.$$

Since $\mathbf{a}_1$ is arbitrary we can drop the subscript, and write for any $\mathbf{a} \in \Omega$

$$\hat{\alpha}_1(\mathbf{a}, t) + \hat{\alpha}_2(\mathbf{q}_2^{-1}(\mathbf{q}_1(\mathbf{a}, t), t)) = 1\,. \tag{6.7}$$

We will see that the function $t \mapsto \mathbf{q}_2^{-1} \circ \mathbf{q}_1(\mathbf{a}, t)$ plays a significant role in the following calculations [D'Avignon et al., 2016]. Let d^3a denote the elementary volume of the mixture at the position $\mathbf{a}$, with d^3r being its corresponding fraction at the position $\mathbf{r}$. As the mass of each phase is preserved in the course of the motion, we can write the following for $k = 1, 2$:

$$\alpha_k(\mathbf{r}, t)\rho_k(\mathbf{r}, t)\,\mathrm{d}^3r = \alpha_k(\mathbf{a}, 0)\rho_k(\mathbf{a}, 0)\,\mathrm{d}^3a\,. \tag{6.8}$$

Recalling (6.3) for mixture mass density in Eulerian form,

$$\rho(\mathbf{r}, t) = \alpha_1(\mathbf{r}, t)\rho_1(\mathbf{r}, t) + \alpha_2(\mathbf{r}, t)\rho_2(\mathbf{r}, t) =: \tilde{\rho}_1(\mathbf{r}, t) + \tilde{\rho}_2(\mathbf{r}, t)\,. \tag{6.9}$$

we can use the Dirac delta-function artifice given in [Morrison, 1998a, Morrison et al., 2020] to obtain the Lagrange to Euler map for $\tilde{\rho}_k = \alpha_k \rho_k$ as follows:

$$\tilde{\rho}_k(\mathbf{r},t) = \alpha_k(\mathbf{r},t)\rho_k(\mathbf{r},t) = \int_\Omega \delta_{\mathbf{r}=\mathbf{q}_k(\mathbf{a},t)}\, \alpha_k(\mathbf{a},0)\rho_k(\mathbf{a},0)\, \mathrm{d}^3a. \tag{6.10}$$

Here $\delta_{\mathbf{r}=\mathbf{q}_k(\mathbf{a},t)} \coloneqq \delta(\mathbf{r}-\mathbf{q}_k(\mathbf{a},t))$ is the delta-function, which upon employing standard manipulations [e.g. Lighthill, 1959] gives

$$\alpha_k(\mathbf{r},t)\rho_k(\mathbf{r},t) = \left.\frac{\alpha_k(\mathbf{a},0)\rho_k(\mathbf{a},0)}{\mathcal{J}_k}\right|_{\mathbf{a}=\mathbf{q}_k^{-1}(\mathbf{r},t)} \tag{6.11}$$

where $\mathcal{J}_k = \det(\partial q_k^i/\partial a^j)$. Hence, the mass of fluid k is conserved along the trajectory $t \to \mathbf{q}_k(\mathbf{a},t)$:

$$\frac{d}{dt}(\hat{\alpha}_k\hat{\rho}_k) = \partial_t(\alpha_k\rho_k) + \nabla\cdot(\alpha_k\rho_k\mathbf{u}_k) = 0. \tag{6.12}$$

where $d(\hat{\alpha}_k\hat{\rho}_k)/dt = 0$, the vanishing derivative at fixed $\mathbf{a}$, follows upon using (6.4) and $\mathcal{J}_k = 1$ at $t = 0$ and the Eulerian mass conservation follows as with the ordinary fluid with $\alpha_k(\mathbf{a},0)\rho_k(\mathbf{a},0)$ replacing $\rho_0(\mathbf{a})$ [cf. Morrison, 1998a]. We will use ∂_t to denote the Eulerian partial derivative at fixed $\mathbf{r}$.

Similarly, if $s_k(\mathbf{a},0)$ is the entropy per unit of mass at time $t = 0$, and we eliminate the thermodynamic interactions between the two phases, the entropy is conserved. We write,

$$s_k(\mathbf{r},t) = s_k(\mathbf{a},0)|_{\mathbf{a}=\mathbf{q}_k^{-1}(\mathbf{r},t)}\,,$$

or upon introducing the entropy density $\sigma_k = \alpha_k\rho_k s_k$. We have,

$$\sigma_k(\mathbf{r},t) = \int_{\Omega_0} \delta_{\mathbf{r}=\mathbf{q}_k(\mathbf{a},t)}\, \sigma_k(\mathbf{a},0)\, \mathrm{d}^3a$$

and upon integrating

$$\sigma_k(\mathbf{r},t) = \left.\frac{\sigma_k(\mathbf{a},0)}{\mathcal{J}_k}\right|_{\mathbf{a}=\mathbf{q}_k^{-1}(\mathbf{r},t)}, \tag{6.13}$$

yielding conservation of σ_k or advection of s_k; viz.,

$$\partial_t\sigma_k + \nabla\cdot(\mathbf{u}_k\,\sigma_k) = 0 \quad \text{or} \quad \partial_t s_k + \mathbf{u}_k\cdot\nabla s_k = 0. \tag{6.14}$$

6.2.1 HAMILTONIAN AND ACTION PRINCIPLE FORMULATION FOR TVM

We now proceed to the Hamiltonian formulation of the TVM, which we obtain by first constructing its action principle in terms of Lagrangian variables.

First, we assume that the mixture is in local thermodynamic equilibrium with independent specific internal energy functions $U_k = U_k(\rho_k, s_k)$. The temperatures and pressures of each phase are given by the usual formulas,

$$T_k = \frac{\partial U_k(\rho_k, s_k)}{\partial s_k} \qquad \text{and} \qquad p_k = \rho_k^2 \frac{\partial U_k(\rho_k, s_k)}{\partial \rho_k} \,. \tag{6.15}$$

Equation (6.15) uses Eulerian variables, with the idea that each Eulerian point $\mathbf{r}$ represents a thermdynamic system. We suppose that the mixture system is bivariant [Benjelloun and Boukharfane, 2021]; this means the mixture energy can be expressed as a function of a single mixture mass density ρ and a mixture specific entropy s, where $\rho = \alpha_1\rho_1 + \alpha_2\rho_2$ and $s = \eta_1 s_1 + \eta_2 s_2$ with the η_k denoting the mass fractions. Because $\eta_1 + \eta_2 = 1$ we write $s = \eta s_1 + (1-\eta)s_2$, where to avoid clutter we set $\eta = \eta_1$.

To find the Hamiltonian formulation, we first obtain the Lagrangian density of the mixture, $\mathcal{L}_{mix}$, and then Legendre transform. Thus, we identify the potential and kinetic energies. In the case of fluids, the potential energy is the internal energy, which stores energy in the form of pressure and temperature. We do not consider gravitational or other interactions. Using the internal energies per unit mass, the total potential energy of the mixture is given by the following formula:

$$\rho U = \alpha_1\rho_1 U_1(\rho_1, s_1) + \alpha_2\rho_2 U_2(\rho_2, s_2) \,, \tag{6.16}$$

or alternatively in terms of the mass fraction as

$$U = \eta U_1(\rho_1, s_1) + (1-\eta) U_2(\rho_2, s_2) \,. \tag{6.17}$$

When construction the Lagrangian density, these must re-expressed in terms of the appropriate Lagrangian variables. Thus, the potential energy for the Lagrangian

density is given by

$$\mathcal{V}\left(\mathbf{q}_1, \frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}, \mathbf{q}_2, \frac{\partial \mathbf{q}_2}{\partial \mathbf{a}}, \hat{\alpha}_1\right) = \rho^0 U = \alpha_1^0 \rho_1^0 U_1\left(\frac{\alpha_1^0 \rho_1^0}{\hat{\alpha}_1 \mathcal{J}_1}, s_1^0\right) + \alpha_2^0 \rho_2^0 U_2\left(\frac{\alpha_2^0 \rho_2^0}{\hat{\alpha}_2 \mathcal{J}_2}, s_2^0\right), \tag{6.18}$$

where we use the shorthand notations $\alpha_k^0 \coloneqq \alpha_k(\mathbf{a}, 0)$, $s_k^0 \coloneqq s_k(\mathbf{a}, 0)$, and $\rho_k^0 \coloneqq \rho(\mathbf{a}, 0)$. Evidently, the kinetic energy density is given by

$$\mathcal{K}(\mathbf{q}_1, \dot{\mathbf{q}}_1 \mathbf{q}_2, \dot{\mathbf{q}}_2) = \mathcal{K}_1 + \mathcal{K}_2 = \frac{1}{2}\alpha_1^0 \rho_1^0 \left|\dot{\mathbf{q}}_1\right|^2 + \frac{1}{2}\alpha_2^0 \rho_2^0 |\dot{\mathbf{q}}_2|^2 . \tag{6.19}$$

Using(6.18) and (6.19), we conclude that the Lagrangian density of the mixture is given by the following:

$$\begin{aligned}\mathcal{L}_{mix}\left(\mathbf{q}_1, \mathbf{q}_2, \dot{q}_1, \dot{\mathbf{q}}_2, \frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}, \frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}, \hat{\alpha}_1\right) &= \mathcal{K} - \mathcal{V} \\ &= \mathcal{L}_1\left(\dot{\mathbf{q}}_1, \mathcal{J}_1, \hat{\alpha}_1\right) + \mathcal{L}_2\left(\dot{\mathbf{q}}_2, \mathcal{J}_2, \hat{\alpha}_2\right) ,\end{aligned} \tag{6.20}$$

where

$$\mathcal{L}_k(\dot{\mathbf{q}}_k, \mathcal{J}_k, \hat{\alpha}_k) = \frac{1}{2}\alpha_k^0 \rho_k^0 \left|\dot{\mathbf{q}}_k\right|^2 - \alpha_k^0 \rho_k^0 U_k\left(\frac{\alpha_k^0 \rho_k^0}{\hat{\alpha}_k \mathcal{J}_k}, s_k^0\right). \tag{6.21}$$

Thus, the Lagrangian is given by

$$L = \int_\Omega \mathcal{L}_{mix}\, \mathrm{d}^3 a = L_1 + L_2. \tag{6.22}$$

and Hamilton's principle amounts to extremizing the action $\int_\Omega L dt$, yielding the Lagrangian equations of motion.

We proceed directly to the Legendre transform, where the momentum densities are given by

$$\boldsymbol{\pi}_k(\mathbf{a}, t) = \frac{\delta L_k}{\delta \dot{\mathbf{q}}_k} = \frac{\partial \mathcal{L}_k}{\partial \dot{\mathbf{q}}_k} = \alpha_k^0 \rho_k^0 \dot{\mathbf{q}}_k \tag{6.23}$$

and the Hamiltonian density is given by

$$\mathcal{H}\left(\mathbf{q}_1, \mathbf{q}_2, \dot{\mathbf{q}}_1, \dot{\mathbf{q}}_2, \frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}, \frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}, \hat{\alpha}_1\right) = \mathcal{H}_1 + \mathcal{H}_2 , \tag{6.24}$$

with

$$\mathcal{H}_k = \boldsymbol{\pi}_k \cdot \dot{\mathbf{q}}_k - \mathcal{L}_k = \frac{1}{2}\alpha_k^0 \rho_k^0 \left|\dot{\mathbf{q}}\right|^2 + \alpha_k^0 \rho_k^0 U_k\left(\frac{\alpha_k^0 \rho_k^0}{\hat{\alpha}_k \mathcal{J}_k}, s_k^0\right). \tag{6.25}$$

Thus the Hamiltonian functional is given by

$$H = \int_\Omega \mathcal{H}\, \mathrm{d}^3a = H_1 + H_2\,. \tag{6.26}$$

Given the above forms of L and H, we arrive at the following:

Theorem 1. *With the boundary conditions $\delta\mathbf{q}_k = 0$ or $\delta\mathbf{q}_k \cdot \mathbf{n} = 0$, for $k = 1, 2$, on the spatial domain $\partial\Omega$, where $\mathbf{n}$ is a unit normal vector, the Lagrangian and Hamiltonian functionals, L and H respectively, depend on the volume fraction if and only if the pressures satisfy $\hat{p}_1 \neq \hat{p}_2\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1}$, which in the Eulerian framework means $p_1 \neq p_2$. Conversely,*

$$\frac{\delta L}{\delta\hat{\alpha}_1} = \frac{\delta H}{\delta\hat{\alpha}_1} = 0 \quad \text{ if and only if } \quad \hat{p}_1 = \hat{p}_2\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1}\,.$$

where the subscript $\mathbf{a} = \mathbf{q}_2^{-1} \circ\ \mathbf{q}_1$ means evaluate the label at the transformed label, i.e.,

$$\hat{p}_1(\mathbf{a}, t) = \hat{p}_2(\mathbf{a}', t)\big|_{\mathbf{a}'=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1(\mathbf{a},t)} = \hat{p}_2(\mathbf{q}_2^{-1} \circ\ \mathbf{q}_1(\mathbf{a}, t), t)\,. \tag{6.27}$$

Proof. To simplify matters we use $\delta_u f = \delta f[u, \delta u]$ for the first variation in u of a functional or a function and here drop the hat on α_1, keeping in mind that it is a Lagrangian variable quantity, i.e., $\alpha_1(\mathbf{a}, t)$. [See, e.g., Morrison, 1998a, for review of functional derivatives and variational calculus]. We have

$$\delta_{\hat{\alpha}_1} L_1 = \int_\Omega \frac{\partial\mathcal{L}_1}{\partial\hat{\alpha}_1}\big(\dot{\mathbf{q}}_1, \mathcal{J}_1, \hat{\alpha}_1, \mathbf{a}\big)\delta\alpha_1\, \mathrm{d}^3a\,,$$

but $\delta_{\alpha_1} L_2$ is more complicated because in the integrand of $L_2\,[\dot{\mathbf{q}}_2, \mathcal{J}_2, \hat{\alpha}_2]$ one must substitute $\mathbf{a} = \mathbf{q}_2^{-1} \circ \mathbf{q}_1(\mathbf{a}', t)$ to align the labels according to (6.5). Thus

$$L_2\,[\dot{\mathbf{q}}_2, \mathcal{J}_2, \hat{\alpha}_2] = \int_\Omega \mathcal{L}_2(\dot{q}_2(\mathbf{a}, t), \mathcal{J}_2(\mathbf{a}, t), 1 - \hat{\alpha}_1(\mathbf{a}', t), \mathbf{a})|_{\mathbf{a}=q_2^{-1}\circ\, q_1(\mathbf{a}', t)}\mathcal{J}_{21}(\mathbf{a}', t)\, \mathrm{d}^3a'\,,$$

where

$$\mathcal{J}_{21}(\mathbf{a}', t) \coloneqq \det\left(\frac{\partial(\mathbf{q}_2^{-1} \circ\ \mathbf{q}_1)}{\partial\mathbf{a}}\right)(\mathbf{a}', t)\,.$$

We obtain

$$\delta_{\hat\alpha_1} L_2 = -\int_\Omega \frac{\partial \mathcal{L}_2}{\partial \alpha_2}\, \big(\dot{\mathbf{q}}_2(\mathbf{a},t), \mathcal{J}_2(\mathbf{a},t), \hat\alpha_2(\mathbf{a},t), \mathbf{a}\big)\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\, \mathbf{q}_1(\mathbf{a}',t)}\, \mathcal{J}_{21}(\mathbf{a}',t)\delta\hat\alpha_1\, \mathrm{d}^3a'$$

and thus

$$\begin{aligned}\delta_{\hat\alpha_1} L = \int_\Omega \Bigg[&\frac{\partial \mathcal{L}_1}{\partial \alpha_1}\big(\dot{\mathbf{q}}_1(\mathbf{a}',t), \mathcal{J}_1(\mathbf{a}',t), \hat\alpha_1(\mathbf{a}',t), \mathbf{a}'\big)\\ &- \frac{\partial \mathcal{L}_2}{\partial \alpha_2}\, \big(\dot{\mathbf{q}}_2(\mathbf{a},t), \mathcal{J}_2(\mathbf{a},t), \hat\alpha_2(\mathbf{a},t), \mathbf{a}\big)\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\, \mathbf{q}_1(\mathbf{a}',t)}\, \mathcal{J}_{21}(\mathbf{a}',t)\Bigg]\, \delta\hat\alpha_1\, \mathrm{d}^3a'\,.\end{aligned}$$

Using

$$\frac{\partial \mathcal{L}_1}{\partial \hat\alpha_1} = -\frac{\partial U_1}{\partial \hat\alpha_1} = \hat p_1 \mathcal{J}_1 \qquad \text{and} \qquad \frac{\partial \mathcal{L}_2}{\partial \hat\alpha_2} = -\frac{\partial U_2}{\partial \hat\alpha_2} = \hat p_2 \mathcal{J}_2\,,$$

we get for all $\mathbf{a}'$ in Ω

$$\begin{aligned}&\frac{\partial \mathcal{L}_2}{\partial \alpha_2}\, \big(\dot{\mathbf{q}}_2(\mathbf{a},t), \mathcal{J}_2(\mathbf{a},t), \hat\alpha_2(\mathbf{a},t), \mathbf{a}\big)\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\, \mathbf{q}_1(\mathbf{a}',t)}\, \mathcal{J}_{21}(\mathbf{a}',t)\\ &= \hat p_2(\mathbf{a},t)\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\, \mathbf{q}_1(\mathbf{a}',t)} \mathcal{J}_2(\mathbf{a},t)\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ \mathbf{q}_1(\mathbf{a}',t)}\, \mathcal{J}_{21}(\mathbf{a}',t) = \hat p_2(\mathbf{a},t)\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\, \mathbf{q}_1(\mathbf{a}',t)} \mathcal{J}_1(\mathbf{a}',t)\,.\end{aligned} \tag{6.28}$$

where in the last equality we used

$$\mathcal{J}_2(\mathbf{a},t)\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\, \mathbf{q}_1(\mathbf{a}',t)}\, \mathcal{J}_{21}(\mathbf{a}',t) = \hat p_2(\mathbf{a},t)\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\, \mathbf{q}_1} \mathcal{J}_1(\mathbf{a}',t)\,.$$

Thus we have a cancellation and can deduce that

$$\begin{aligned}&\frac{\delta L}{\delta \hat\alpha_1} = 0 \quad \text{if and only if} \quad \hat p_1(\mathbf{a}',t)\mathcal{J}_1(\mathbf{a}',t) = \hat p_2(\mathbf{a},t)\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ \mathbf{q}_1(\mathbf{a}',t)} \mathcal{J}_1(\mathbf{a}',t)\,,\\ &\qquad\qquad \text{i.e.} \quad \hat p_1 = \hat p_2\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\, \mathbf{q}_1}.\end{aligned} \tag{6.29}$$

□

This theorem will be instrumental in the development below and in re-interpreting some results in the literature. Now we proceed to obtain the equations of motion for the TVM using the Hamiltonian form. Let

$$\boldsymbol{\pi} \coloneqq \begin{pmatrix} \boldsymbol{\pi}_1 \\ \boldsymbol{\pi}_2 \end{pmatrix} \qquad \text{and} \qquad \mathbf{q} \coloneqq \begin{pmatrix} \mathbf{q}_1 \\ \mathbf{q}_2 \end{pmatrix} \tag{6.30}$$

where, $\boldsymbol{\pi}_k(\mathbf{a},t) = \delta L/\delta\dot{\mathbf{q}}_k = \alpha_k^0\rho_k^0\dot{\mathbf{q}}_k$. If we take the matrix $\mathbf{A} = \left(\frac{\partial q_i}{\partial a_j}\right)_{i,j}$, we have:

$$\mathbf{A}^{-1} = \frac{1}{\mathbf{det}(A)}\ {}^tCom(\mathbf{A}) = \frac{1}{\mathcal{J}}\ {}^tCom(\mathbf{A}) = (\Delta_i^j)_{i,j}.$$

We present a list of useful formulas to complete the proof:

$$\frac{\partial}{\partial q^i} = \frac{1}{\mathcal{J}}\Delta_i^j\frac{\partial}{\partial a^j}. \tag{6.31}$$

$$\Delta_i^j = \frac{\partial\mathcal{J}}{\partial\left(\partial q^i/\partial a^j\right)} \tag{6.32}$$

$$\delta\mathcal{J} = \Delta_i^k\frac{\partial\delta q_i}{\partial a_k} \quad \text{Or} \quad \dot{\mathcal{J}} = \Delta_i^k\frac{\partial\dot{q}_i}{\partial a_k} \tag{6.33}$$

The Hamiltonian functional is given by (6.26), with densities (6.24) and (6.25). With the boundary conditions defined in Theorem 1 we get

$$\frac{\delta H_1}{\delta q_1^i} = \frac{\partial\mathcal{H}_1}{\partial q_1^i} - \frac{\partial}{\partial a_j}\frac{\partial\mathcal{H}_1}{\partial(\partial q_1^i/\partial a^j)}\,. \tag{6.34}$$

The first term of (6.34) is zero, while the second we apply the result of (6.31)-(6.32) we get:

$$\begin{aligned}
\frac{\partial}{\partial a^j}\frac{\partial\mathcal{H}_1}{\partial(\partial q_1^i/\partial a^j)} &= \frac{\partial}{\partial a^j}\frac{\partial(\alpha_1^0\rho_1^0U_1(\frac{\tilde{\rho}_1^0}{\hat{\alpha}_1\mathcal{J}}, s_1^0))}{\partial(\partial q_1^i/\partial a^j)} \\
&= \Delta_i^j\frac{\partial}{\partial a^j}\frac{\partial(\alpha_1^0\rho_1^0U_1(\frac{\tilde{\rho}_1^0}{\hat{\alpha}_1\mathcal{J}}, s_1^0))}{\partial\mathcal{J}}, \\
&= -\Delta_i^j\frac{\partial}{\partial a^j}\left(\frac{1}{\mathcal{J}^2}\frac{\alpha_1^0\rho_1^0\tilde{\rho}_1^0}{\hat{\alpha}_1}\frac{\partial U_1}{\partial\rho_1}(\hat{\rho}_1, s_1^0)\right) \\
&= -\mathcal{J}_1\frac{\partial}{\partial q_1^i}(\hat{\alpha}_1\rho_1^2\frac{\partial U_1}{\partial\rho_1})
\end{aligned}$$

where recall $\tilde{\rho}_1^0 = \alpha_1^0\rho_1^0$ and here the co-factor matrix is $\Delta_i^j = \frac{1}{2}\epsilon_{ikl}\,\epsilon^{jmn}\,\frac{\partial q^k}{\partial a^m}\frac{\partial q^l}{\partial a^n}$, with the Levi-Civita permutation symbol given as usual by

$$\epsilon_{ijk} = \begin{cases} 1 & \text{if} \quad (i\,j\,k) \quad \text{is a cyclic permutation} \\ -1 & \text{if} \quad (i\,j\,k) \quad \text{is an anti-cyclic permutation} \\ 0 & \text{if} \quad i=j=k \end{cases}.$$

Since $\hat{\alpha}_2$ depends on $\mathbf{q}_1$, by the formula $\hat{\alpha}_1 + \hat{\alpha}_2|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1} = 1$. So we must

calculate the quantity $\delta\mathcal{H}_2/\delta q_1^i$ which is not expected to vanish, i.e.,

$$\delta_{\mathbf{q}_1} H_2 = \int_\Omega \delta_{\mathbf{q}_1}\mathcal{H}_2\left(\mathbf{q}_2, \frac{\partial \mathbf{q}_2}{\partial \mathbf{a}}, \hat{\alpha}_2\right) d^3a = \int_\Omega \frac{\partial}{\partial \hat{\alpha}_2}\mathcal{H}_2\left(\mathbf{q}_2, \frac{\partial \mathbf{q}_2}{\partial \mathbf{a}}, \hat{\alpha}_2\right) \delta_{\mathbf{q}_1}\hat{\alpha}_2\, d^3a$$

But writing that,

$$\hat{\alpha}_2(\mathbf{a}, t) = 1 - \hat{\alpha}_1\left(\mathbf{q}_1^{-1}\left(\mathbf{q}_2(\mathbf{a}, t)\right), t\right),$$

we obtain

$$\delta_{\mathbf{q}_1}\hat{\alpha}_2(\mathbf{a}, t) = -\frac{\partial \hat{\alpha}_1}{\partial \mathbf{a}}\big(\mathbf{q}_1^{-1} \circ\ \mathbf{q}_2(\mathbf{a}, t), t\big)\, \delta_{\mathbf{q}_1}\left(\mathbf{q}_1\right)^{-1}\left(\mathbf{q}_2(\mathbf{a}, t), t\right).$$

We get then

$$\delta_{\mathbf{q}_1}\hat{\alpha}_2\big(\mathbf{q}_2^{-1} \circ\ \mathbf{q}_1(\mathbf{a}, t), t\big) = \frac{\partial \hat{\alpha}_1}{\partial \mathbf{a}}(\mathbf{a}, t)\left(\frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}\right)^{-1}(\mathbf{a}, t)\delta\mathbf{q}_1(\mathbf{a}, t). \tag{6.35}$$

We may then write that,

$$\begin{aligned}
\delta_{\mathbf{q}_1} H_2 &= \int_\Omega \frac{\partial \mathcal{H}_2}{\partial \hat{\alpha}_2}\left(\dot{\mathbf{q}}_2, \mathcal{J}_2, \hat{\alpha}_2, \mathbf{a}\right)\delta_{\mathbf{q}_1}\hat{\alpha}_2\, d^3a \\
&= \int_\Omega \left[\frac{\partial \mathcal{H}_2}{\partial \hat{\alpha}_2}\left(\dot{\mathbf{q}}_2, \mathcal{J}_2, \hat{\alpha}_2, \mathbf{a}\right)\delta_{\mathbf{q}_1}\alpha_2\right]_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1} \det\left(\frac{\partial(\mathbf{q}_2^{-1} \circ\ \mathbf{q}_1)}{\partial \mathbf{a}}\right) d^3a \\
&= \int_\Omega \left\{\left[\frac{\partial \mathcal{H}_2}{\partial \hat{\alpha}_2}\left(\dot{\mathbf{q}}_2, \mathcal{J}_2, \hat{\alpha}_2, \mathbf{a}\right)\right]_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1} \frac{\partial \hat{\alpha}_1}{\partial \mathbf{a}}\left(\frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}\right)^{-1}\mathcal{J}_{21}\right\}\delta\mathbf{q}_1\, d^3a\,.
\end{aligned}$$

Hence,

$$\frac{\delta H_2}{\delta \mathbf{q}_1} = \left.\frac{\partial \mathcal{H}_2}{\partial \hat{\alpha}_2}\right|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1} \frac{\partial \hat{\alpha}_1}{\partial \mathbf{a}}\left(\frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}\right)^{-1}\mathcal{J}_{21}.$$

On the other side, we have

$$\frac{\partial \mathcal{H}_2}{\partial \hat{\alpha}_2} = -\frac{\partial \mathcal{L}_2}{\partial \hat{\alpha}_2} = \frac{\partial U_2}{\partial \hat{\alpha}_2} = -\hat{p}_2\mathcal{J}_2.$$

We develop our calculations,

$$\begin{aligned}
\frac{\delta H_2}{\delta \mathbf{q}_1} = \left.\frac{\partial \mathcal{H}_2}{\partial \hat{\alpha}_2}\right|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1} \frac{\partial \hat{\alpha}_1}{\partial \mathbf{a}}\left(\frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}\right)^{-1}\mathcal{J}_{21} &= -\hat{p}_2|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1}\mathcal{J}_2|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1}\mathcal{J}_{21}\frac{\partial \hat{\alpha}_1}{\partial \mathbf{a}}\left(\frac{\partial \mathbf{q}_1}{\partial \mathbf{a}}\right)^{-1} \\
&= -\hat{p}_2|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1}\mathcal{J}_1\frac{\partial \hat{\alpha}_1}{\partial \mathbf{a}}\left(\frac{\partial q_1}{\partial \mathbf{a}}\right)^{-1}.
\end{aligned}$$

Hamilton's equations imply,

$$\alpha_1^0\rho_1^0\,\ddot{q}_{1i} = \hat{p}_2\big|_{\mathbf{a}=\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1}\mathcal{J}_1\frac{\partial\hat{\alpha}_1}{\partial q_1^i} - \mathcal{J}_1\frac{\partial}{\partial q_1^i}\left(\hat{\alpha}_1\rho_1^2\frac{\partial U_1}{\partial\rho_1}\right) \tag{6.36}$$

and in a symmetrical way we also find

$$\alpha_2^0\rho_2^0\,\ddot{q}_{2i} = \hat{p}_1\big|_{\mathbf{a}=\mathbf{q}_1^{-1}\circ\,\mathbf{q}_2}\mathcal{J}_2\frac{\partial\hat{\alpha}_2}{\partial q_2^i} - \mathcal{J}_2\frac{\partial}{\partial q_2^i}\left(\hat{\alpha}_2\rho_2^2\frac{\partial U_2}{\partial\rho_2}\right). \tag{6.37}$$

It is difficult to treat the equation in its Lagrangian form and, in any event, the Eulerian framework is required. We appeal to the Theorem (1). We suppose firstly that the Hamiltonian does not depend of parameter α. Then we assume that $\hat{p}_1 = \hat{p}_2\big|_{\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1}$. Hence the equations of motion for become:

$$\alpha_k^0\rho_k^0\,\ddot{q}_{2i} = -\mathcal{J}_k\hat{\alpha}_k\frac{\partial}{\partial q_k^i}\left(\hat{\alpha}_k\rho_k^2\frac{\partial U_k}{\partial\rho_k}\right). \tag{6.38}$$

The obtained equations (6.12), (6.14), (6.36), and (6.38)) can be transformed into Eulerian form [Morrison, 1998a]

$$\partial_t(\alpha_k\rho_k) = -\nabla\cdot(\alpha_k\rho_k\mathbf{u}_k)\,, \tag{6.39}$$

$$\partial_t(\alpha_k\rho_k\mathbf{u}_k) = -\nabla\cdot(\alpha_k\rho_k\mathbf{u}_k\otimes\mathbf{u}_k) - \alpha_k\nabla p\,, \tag{6.40}$$

$$\partial_t s_k = -\mathbf{u}_k\cdot\nabla s_k\,, \tag{6.41}$$

with $p_1 = p_2 = p$ and $\alpha_2 = 1-\alpha_1$.

Upon transforming (6.39), (6.40), and (6.41) from the variables $(\alpha_1,\rho_1,\rho_2,\mathbf{u}_1,\mathbf{u}_2,s_1,s_2)$ to the variables $(\alpha_1,p,\mathbf{u}_1,\mathbf{u}_2,s_1,s_2)$ we obtain following form:

$$\begin{aligned} e\,\partial_t\alpha_1 = &-\alpha_1\alpha_2(\mathbf{u}_1-\mathbf{u}_2)\cdot\nabla p - \alpha_1\alpha_2c_1^2\rho_1\nabla\cdot\mathbf{u}_1 \\ &+\alpha_1\alpha_2c_2^2\rho_2\nabla\cdot\mathbf{u}_2 - \left[\alpha_2\rho_1\mathbf{u}_1c_1^2+\alpha_1\rho_2\mathbf{u}_2c_2^2\right]\cdot\nabla\alpha_1\,, \end{aligned} \tag{6.42}$$

$$\begin{aligned} e\,\partial_t p = &-(\alpha_1\rho_2c_2^2\mathbf{u}_1+\alpha_2\rho_1c_1^2\mathbf{u}_2)\cdot\nabla p \\ &-\alpha_1\rho_1\rho_2c_2^2c_1^2\nabla\cdot\mathbf{u}_1 - \alpha_2\rho_1\rho_2c_1^2c_2^2\nabla\cdot\mathbf{u}_2 \\ &-\left[\rho_1\rho_2c_2^2c_1^2\mathbf{u}_1-\rho_1\rho_2c_1^2c_2^2\mathbf{u}_2\right]\cdot\nabla\alpha_1\,, \end{aligned} \tag{6.43}$$

$$\partial_t\mathbf{u}_k = -\mathbf{u}_k\cdot\nabla\mathbf{u}_k - \frac{1}{\rho_k}\nabla p\,, \tag{6.44}$$

$$\partial_t s_k = -\mathbf{u}_k\cdot\nabla s_k\,, \tag{6.45}$$

where $e \coloneqq \alpha_1c_2^2\rho_2+\alpha_2c_1^2\rho_1$ is an energy-like quantity and c_k is the sound speed of

the phase k, i.e., $c_k^2 = \partial p_k/\partial \rho_k|_{s_k}$.

6.2.2 STABILITY AND HYPERBOLICITY OF THE TVM SYSTEM

In this section, we address the stability and hyperbolicity of the TVM System. Upon linearizing around constant values of $(\alpha_1, p, u_1, u_2, s_1, s_2)$, the TVM system in one dimension becomes

$$\partial_t U + A\,\partial_x U = 0\,, \tag{6.46}$$

where $U = (\tilde{\alpha}_1, \tilde{p}, \tilde{u}_1, \tilde{u}_2, \tilde{s}_1, \tilde{s}_2)$ is the deviation for the equilibrium state and

$$A = \frac{1}{e}\begin{bmatrix} \alpha_1 c_2^2\rho_2 u_2 + \alpha_2 c_1^2\rho_1 u_1 & \alpha_1\alpha_2(u_1-u_2) & \alpha_1\alpha_2 c_1^2\rho_1 & -\alpha_1\alpha_2 c_2^2\rho_2 & 0 & 0 \\ c_1^2c_2^2\rho_1\rho_2\,(u_1-u_2) & \alpha_1 c_2^2\rho_2 u_1 + \alpha_2 c_1^2\rho_1 u_2 & \alpha_1 c_1^2 c_2^2\rho_1\rho_2 & \alpha_2 c_1^2 c_2^2\rho_1\rho_2 & 0 & 0 \\ 0 & e/\rho_1 & eu_1 & 0 & 0 & 0 \\ 0 & e/\rho_2 & 0 & eu_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & eu_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & eu_2 \end{bmatrix}$$

where recall $e \coloneqq \alpha_1 c_2^2\rho_2 + \alpha_2 c_1^2\rho_1$.

Lemma 4. *The matrix A has six real distinct eigenvalues if and only if,*

$$(u_1-u_2)^2 \geq \frac{c_1^2c_2^2}{\alpha_2\rho_1c_1^2 + \alpha_1\rho_2c_2^2}\left[(\rho_1\alpha_2)^{1/3} + (\rho_2\alpha_1)^{1/3}\right]^3. \tag{6.47}$$

The condition (6.47) is given to ensure the hyperbolicity of the linear TVM System [Stewart and Wendroff, 1984]. We can prove that the hyperbolicity is equivalent to the stability in the sense of von Neumann [Hicks, 1981, Ransom and Hicks, 1984, 1988]. Moreover, using the theorems presented in [Kreiss and Lorenz, 2004, see page 102], we can prove that this condition implies the strong solution existence of the Linear TVM system with a given initial data.

Remark 1. *We recovered in the above development the well-known TVM for two-phase flows. However, in Theorem 1 we have shown that the single pressure hypothesis, $\hat{p}_1(\mathbf{a},t) = \hat{p}_2|_{\mathbf{q}_2^{-1}\circ\,\mathbf{q}_1}(\mathbf{a},t)$ (i.e $p_1(\mathbf{r},t) = p_2(\mathbf{r},t)$), is necessary to derive this model. This limitation is not always respected in the literature [Drui et al., 2019, Holm and Kupershmidt, 1986, Hicks, 1981, Stewart and Wendroff, 1984]. Many models assume different phase pressures yet present equations of the form of the*

TVM here. If we suppose in this model that $\mathbf{u}_1 = \mathbf{u}_2 = \mathbf{u}$*, then the momentum conservation equations become*

$$\mathbf{u}_t = -\mathbf{u}\cdot\nabla\mathbf{u} - \frac{1}{\rho_1}\nabla p\,, \tag{6.48}$$

$$\mathbf{u}_t = -\mathbf{u}\cdot\nabla\mathbf{u} - \frac{1}{\rho_2}\nabla p\,. \tag{6.49}$$

By identification, we get that $\rho_1 = \rho_2$*. So a mixture of two different phases* ($\rho_1 \neq \rho_2$) *with one pressure cannot flow with the same velocities.*

If we take into account the viscosity, we must add to the momentum conservation and entropy equations terms depending on the viscosities μ_k as follows:

$$\partial_t(\alpha_k\rho_k) = -\nabla\cdot(\alpha_k\rho_k\mathbf{u}_k)\,, \tag{6.50}$$

$$\partial_t(\alpha_k\rho_k\mathbf{u}_k) = -\nabla\cdot(\alpha_k\rho_k\mathbf{u}_k\otimes\mathbf{u}_k) - \alpha_k\nabla p + \nabla\cdot(\alpha_k\mu_k\nabla\mathbf{u}_k)\,, \tag{6.51}$$

$$\partial_t s_k = -\mathbf{u}_k\cdot\nabla s_k + \frac{\mu_k}{\rho_k T_k}\nabla\mathbf{u}_k : \nabla\mathbf{u}_k\,, \tag{6.52}$$

We call the above system with viscosities the real Two-Velocity Model (rTVM).

6.2.3 WAVE BEHAVIOR IN RTVM

Now consider linear sound waves in the rTVM (6.50)-(6.52). We add the effect due to viscosity of each fluid (μ_1, μ_2) and we simplify the model [see Benjelloun and Zaidni, 2021, Stewart and Wendroff, 1984]. The system of equation with viscosity can be summarized as follows:

$$\begin{aligned} e\,\partial_t\alpha_1 = &-\alpha_1\alpha_2(\mathbf{u}_1-\mathbf{u}_2)\cdot\nabla p - \alpha_1\alpha_2 c_1^2\rho_1\nabla\cdot\mathbf{u}_1 \\ &+ \alpha_1\alpha_2 c_2^2\rho_2\nabla\cdot\mathbf{u}_2 - \left(\alpha_2\rho_1\mathbf{u}_1 c_1^2 + \alpha_1\rho_2\mathbf{u}_2 c_2^2\right)\cdot\nabla\alpha_1 \\ &+ \alpha_1\alpha_2\Gamma_1\mu_1\nabla\mathbf{u}_1 : \nabla\mathbf{u}_1 - \alpha_1\alpha_2\Gamma_2\mu_2\nabla\mathbf{u}_2 : \nabla\mathbf{u}_2\,, \end{aligned} \tag{6.53}$$

$$\begin{aligned} e\,\partial_t p = &-(\alpha_1\rho_2 c_2^2\mathbf{u}_1 + \alpha_2\rho_1 c_1^2\mathbf{u}_2)\cdot\nabla p - \alpha_1\rho_1\rho_2 c_2^2 c_1^2\nabla\cdot\mathbf{u}_1 \\ &- \alpha_2\rho_1\rho_2 c_1^2 c_2^2\nabla\cdot\mathbf{u}_2 - \left(\rho_1\rho_2 c_2^2 c_1^2\mathbf{u}_1 - \rho_1\rho_2 c_1^2 c_2^2\mathbf{u}_2\right)\cdot\nabla\alpha_1 \\ &+ \alpha_1\rho_2 c_2^2\Gamma_1\mu_1\nabla\mathbf{u}_1 : \nabla\mathbf{u}_1 + \alpha_2\rho_1 c_1^2\Gamma_2\mu_2\nabla\mathbf{u}_2 : \nabla\mathbf{u}_2\,, \end{aligned} \tag{6.54}$$

$$\partial_t\mathbf{u}_k = -\mathbf{u}_k\cdot\nabla\mathbf{u}_k + \frac{1}{\rho_k}\nabla p + \frac{\mu_k}{\alpha_k\rho_k}\nabla\alpha_k\cdot\nabla\mathbf{u}_k + \frac{\mu_k}{\rho_k}\Delta\mathbf{u}_k\,, \tag{6.55}$$

$$\partial_t s_k = -\mathbf{u}_k\cdot\nabla s_k + \frac{\mu_k}{\rho_k T_k}\nabla\mathbf{u}_k : \nabla\mathbf{u}_k\,. \tag{6.56}$$

After the linearization of the system (6.53)-(6.56) in one-dimensional around a constant solution
$(\alpha_1, p, u_1 \approx 0, u_2 \approx 0, s_1, s_2)$. We look for non-zero harmonic plane-wave solutions for $U = (\alpha_1, p, u_1, u_1, s_1, s_2)$ of the form

$$U = U_0 \exp(i\omega t + kx) = U_0 \exp(k_R x) \exp\left(i(\omega t + k_I x)\right), \tag{6.57}$$

where ω is the sound frequency and $k = k_R + ik_I$ is a complex wavelength, that contains the wavelength k_I and the attenuation k_R. Thus we are led to the following:

$$(\omega I - ikA + ik^2 B) \cdot U = 0\,, \tag{6.58}$$

where I is the identity matrix and

$$A = \frac{1}{e} \begin{bmatrix} 0 & 0 & \alpha_1\alpha_2 c_1^2 \rho_1 & -\alpha_1\alpha_2 c_2^2 \rho_2 & 0 & 0 \\ 0 & 0 & \alpha_1 c_1^2 c_2^2 \rho_1\rho_2 & \alpha_2 c_1^2 c_2^2 \rho_1\rho_2 & 0 & 0 \\ 0 & e/\rho_1 & 0 & 0 & 0 & 0 \\ 0 & e/\rho_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{6.59}$$

and

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mu_1/\rho_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu_2/\rho_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{6.60}$$

Hence, upon setting the determinant $\det(\omega I - ikA + ik^2 B)$ to zero, we get the dispersion relation

$$1 + E\left(\frac{k}{\omega}\right)^2 + F\left(\frac{k}{\omega}\right)^4 = 0\,, \tag{6.61}$$

where

$$F = c_\infty^4 \left[i \frac{\alpha_1\mu_2 + \alpha_2\mu_1}{\alpha_1\rho_2 + \alpha_2\rho_1} \frac{\omega}{c_\infty^2} - \frac{\mu_1\mu_2\omega^2}{\rho_1\rho_2 c_\infty^4} \right], \tag{6.62}$$

$$E = c_\infty^2 \left[1 + i \left(\frac{\alpha_1\mu_1\rho_2}{\rho_1\, c_1^2} + \frac{\alpha_2\mu_2\rho_1}{\rho_2\, c_2^2} \right) \frac{\omega}{\alpha_1\rho_2 + \alpha_2\rho_1} \right. \\ \left. + i \left(\frac{\alpha_1\mu_2}{c_1^2} + \frac{\alpha_2\mu_1}{c_2^2} \right) \frac{\omega}{\alpha_1\rho_2 + \alpha_2\rho_1} \right], \tag{6.63}$$

$$c_\infty = \frac{\omega}{k} = \sqrt{\frac{\alpha_2\rho_1 c_1^2 c_2^2 + \alpha_1\rho_2 c_1^2 c_2^2}{\alpha_1\rho_2 c_2^2 + \alpha_2\rho_1 c_1^2}}\,. \tag{6.64}$$

The velocity c_∞ represents the speed of propagation of the wave (when $\mu_1 = \mu_2 = 0$). Using the following definitions:

$$\bar\rho = \alpha_1\rho_2 + \alpha_2\rho_1, \qquad \bar\mu = \alpha_1\mu_2 + \alpha_1\mu_1, \qquad \beta_1 = \frac{\alpha_1\rho_2}{\bar\rho}\,. \\ \beta_2 = \frac{\alpha_2\rho_1}{\bar\rho}, \qquad \beta_1 + \beta_2 = 1\,, \tag{6.65}$$

and the Knudsen numbers

$$K_1 = \frac{\mu_1\omega}{\rho_1 c_1^2}, \qquad K_2 = \frac{\mu_2\omega}{\rho_2 c_2^2}, \quad K_n = \frac{\bar\mu\omega}{\bar\rho c_\infty^2}, \\ K_{1,2} = \left(\frac{\alpha_1\mu_2}{c_1^2} + \frac{\alpha_2\mu_1}{c_2^2} \right) \frac{\omega}{\bar\rho}, \quad K_m = \frac{\omega}{c_\infty^2} \sqrt{\frac{\mu_1\mu_2}{\rho_1\rho_2}}\,, \tag{6.66}$$

the dispersion relation becomes a bi-quadratic polynomial

$$1 + \left[1 + i\beta_1 K_1 + i\beta_2 K_2 + i K_{1,2} \right] \left(\frac{k c_\infty}{\omega} \right)^2 + (iK_n - K_m^2) \left(\frac{k c_\infty}{\omega} \right)^4 = 0\,. \tag{6.67}$$

Next, assuming that $K_1, K_2, K_{1,2}, K_n, K_m \ll 1$, we obtain to second order that the discriminant of the bi-quadratic polynomial is given by

$$\sqrt{\Delta} = \pm \left[1 + i(\beta_1 K_1 + \beta_2 K_2 + K_{1,2}) - 2(iK_n - K_m^2)^2 \right]\,,$$

with the complex wavelengths solutions given by

$$k^\pm = \frac{1}{\lambda^\pm} = \pm \frac{i\omega}{c_\infty} \left[1 + \frac{1}{8} \left(\beta_1 K_1 + \beta_2 K_2 + K_{1,2} \right)^2 + \frac{1}{2} K_n^2 + \frac{i}{2} (\beta_1 K_1 + \beta_2 K_2 + K_{1,2}) \right].$$

Then, the expressions for dispersion and attenuation at order 2 in the Knudsen

numbers are

$$v_s(\omega) = \frac{\omega}{Im(k)} \approx c_\infty \left(1 + \frac{1}{8}\left(\beta_1 K_1 + \beta_2 K_2 + K_{1,2}\right)^2 + \frac{1}{2}K_n^2\right), \tag{6.68}$$

$$\alpha(\omega) = Re(k) \approx -\frac{\omega}{2c_\infty}(\beta_1 K_1 + \beta_2 K_2 + K_{1,2})\,. \tag{6.69}$$

In the following subsection, we present some hypothesis that allow us to close our system by expressing an equation between the pressures of each phase. This is obligatory because the phases are not fully independent and, because of our Remark 1, the pressures $\hat{p}_2|_{\mathbf{q}_2^{-1}\circ\mathbf{q}_1}$ and $\hat{p}_1$ should not be equal.

6.2.4 SURFACE TENSION: LAPLACE'S LAW

Laplace's Law is an equation that describes the capillary pressure difference sustained across the interface between two phases, such as water and air, due to the phenomenon of surface tension or wall tension. For example, In the case of dispersed flows, we have either the gas bubbles in the liquid, or liquid droplets in gas. Both cases assume we have in the mixture spheres of radius R. The pressures of the phases is related to the radius and the surface tension σ by the formula

$$p_2 - p_1 = \frac{2\sigma}{R} = \epsilon\,, \tag{6.70}$$

where p_1 is the pressure inside of a sphere of the phase "1" and p_2 is the pressure outside. First, we assume that the balls have the same radius (R =constant, monodispersed flow). From our previous explanations (1), we must note that necessarily $\sigma \neq 0$.

In this case as $\partial_t p_1 = \partial_t p_2$, and $\nabla p_1 = \nabla p_2$. In one-dimensional, the equations (6.12), (6.14), (6.36), and (6.37)) take the following Eulerian form:

$$\partial_t U + A\partial_x U = 0\,, \tag{6.71}$$

where

$$A = \frac{1}{e}\begin{bmatrix} \alpha_1 c_2^2\rho_2 u_2 + \alpha_2 c_1^2\rho_1 u_1 & \alpha_1\alpha_2(u_1-u_2) & \alpha_1\alpha_2 c_1^2\rho_1 & -\alpha_1\alpha_2 c_2^2\rho_2 & 0 & 0 \\ c_1^2c_2^2\rho_1\rho_2\,(u_1-u_2) & \alpha_1 c_2^2\rho_2 u_1 + \alpha_2 c_1^2\rho_1 u_2 & \alpha_1 c_1^2c_2^2\rho_1\rho_2 & \alpha_2 c_1^2c_2^2\rho_1\rho_2 & 0 & 0 \\ -\epsilon e/(\alpha_1\rho_1) & e/\rho_1 & eu_1 & 0 & 0 & 0 \\ \epsilon e/(\alpha_2\rho_2) & e/\rho_2 & 0 & eu_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & eu_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & eu_2 \end{bmatrix}.$$

The above matrix has the following characteristic polynomial:

$$\mathcal{P}_A = (x-u_1)(x-u_2)\mathcal{X}_A\,, \tag{6.72}$$

where

$$\mathcal{X}_A = (\phi-\delta)^2(\phi+\delta)^2 - e\mathcal{M}_1(\phi-\delta)^2 - e\mathcal{M}_2(\phi+\delta)^2 + e\mathcal{M}_3,$$

with $\phi = x - \frac{1}{2}(u_1+u_2)$, $\delta = (u_1-u_2)/2$ and

$$\mathcal{M}_1 = \epsilon\alpha_1 c_2^2 + c_1^2c_2^2\alpha_2\rho_1\,, \quad \mathcal{M}_2 = -\epsilon\alpha_2 c_1^2 + c_1^2c_2^2\alpha_1\rho_2\,, \quad \mathcal{M}_3 = c_1^2c_2^2\epsilon(\alpha_1-\alpha_2)\,.$$

Now, if ($u_1 \approx u_2 \approx 0$), the characteristic polynomial of the matrix A is bi-quadratic,

$$\mathcal{P}_A = x^2\left(x^4 + \frac{\epsilon\bar{c}^2 - c_1^2c_2^2\bar{\rho}}{e}x^2 - \frac{\epsilon c_1^2c_2^2}{e}\right). \tag{6.73}$$

where $\bar{c}^2 = \alpha_1 c_2^2 + \alpha_2 c_1^2$. Thus the matrix has 4 non-zero eigenvalues,

$$\lambda_{1,2,3,4} = \pm\sqrt{\frac{c_1^2c_2^2\bar{\rho} - \epsilon\bar{c}^2}{2e} \pm \frac{\sqrt{\Delta}}{2}}\,, \tag{6.74}$$

where Δ is the discriminant of the bi-quadratic polynomial $\mathcal{X}_A$. The two eigenvalues

$$\lambda_{1,2} = \pm\sqrt{\left(\frac{c_1^2c_2^2\bar{\rho} - \epsilon\bar{c}^2}{2e} + \frac{\sqrt{\Delta}}{2}\right)}$$

are real and represent the sound speed c_ϵ^∞. The others

$$\lambda_{3,4} = \pm\sqrt{\left(\frac{c_1^2c_2^2\bar{\rho} - \epsilon\bar{c}^2}{2e} - \frac{\sqrt{\Delta}}{2}\right)}$$

are pure imaginary complex numbers. We have that, $|\lambda_{1,2}|(\alpha_1 \to 0) = c_2$ and

$|\lambda_{1,2}|(\alpha_2 \to 0) = c_1$. A common example of use is finding the pressure inside an air bubble in pure water, where $\sigma = 72mN/m$ at 25 $°C\,(298K)$. The extra pressure inside the bubble is given here for three bubble sizes:

Bubble diameter $(2r)(\mu\text{m})$	$\Delta P(\text{ Pa})$	$\Delta P(\text{ atm})$
1000	288	0.00284
3.0	96000	0.947
0.3	960000	9.474

If we take into account the viscosity, the same method as before gives dispersion and attenuation formulas to order 2 at Knudsen numbers:

$$v_s(\omega) \approx c_\epsilon^\infty \left(1 + \frac{1}{8}k_\epsilon^2 + \frac{1}{2}K_{n,\epsilon}^2\right), \qquad \alpha(\omega) \approx -\frac{\omega}{2c_\epsilon^\infty}K_\epsilon\,,$$

where

$$\begin{aligned}
\tilde{C}_\infty &= \sqrt{\frac{c_1^2c_2^2\bar{\rho} - \epsilon\bar{c}^2}{\alpha_1c_2^2\rho_2 + \alpha_2c_1^2\rho_1}}, \qquad G = \frac{\epsilon c_1^2c_2^2}{\tilde{C}_\infty^4 e}\,,\\
K_\epsilon &= \frac{\omega}{\sqrt{1+4G}}\left(\frac{\alpha_1c_2^2\mu_1\rho_2^2 + \alpha_2c_1^2\mu_2\rho_1^2}{\tilde{C}_\infty^2 e\rho_1\rho_2} + \frac{\alpha_1c_2^2\mu_2 + \alpha_2c_1^2\mu_1}{\tilde{C}_\infty^2 e}\right),\\
K_{n,\epsilon} &= \frac{\omega}{1+4G+\sqrt{1+4G}}\left(\frac{\bar{\mu}c_1^2c_2^2}{\tilde{C}_\infty^4 e} - \frac{\epsilon(\alpha_1c_2^2\mu_1\rho_2 + \alpha_2c_1^2\mu_2\rho_1)}{\tilde{C}_\infty^4 e\rho_1\rho_2}\right).
\end{aligned} \tag{6.75}$$

Remark 2. *The characteristic polynomial* (6.72) *has complex roots and the system is non-hyperbolic.*

6.3 ONE VELOCITY MODEL (ZDFM)

In this section we treat a special case of the previous model and where $\mathbf{q}_1 = \mathbf{q}_2$. The particles of each constituent are in the initial position $\mathbf{a} \in \Omega$, and then at the time t they a re located at $\mathbf{r} = \mathbf{q}(\mathbf{a}, t) = \mathbf{q}_1(\mathbf{a}, t) = \mathbf{q}_2(\mathbf{a}, t)$. In the case of one velocity models/flows, we have one common velocity field noted $\mathbf{u}(r, t) = \dot{\mathbf{q}}_1(\mathbf{a}, t)|_{\mathbf{a}=\mathbf{q}_1^{-1}(\mathbf{r},t)} = \dot{\mathbf{q}}_2(\mathbf{a}, t)|_{\mathbf{a}=\mathbf{q}_2^{-1}(\mathbf{r},t)}$ and also one Jacobian matrix $\mathcal{J}_1 = \mathcal{J}_2 = \mathcal{J}$.

In the Eulerian picture, equation of motion reads,

$$\partial_t(\rho\,\mathbf{u}) + \nabla\cdot(\rho\,\mathbf{u}\otimes\mathbf{u}) = (p_2 - p_1)\nabla\alpha_1 - \nabla(\alpha_1p_1 + \alpha_2p_2). \tag{6.76}$$

We suppose that $p_2 = p_1$, we fall into the case of a simple fluid of density $\rho = \alpha_1\rho_1 + \alpha_2\rho_2$. Just the equations of state that change. In this case we have the conservation of the mass fraction,

$$\partial_t \eta + u \cdot \nabla \eta = 0. \tag{6.77}$$

which did not appear in the TVM model. The equation of state for the pressure is written as $p = P(\rho, \eta, s_1, s_2)$, with $p = p_1 = p_2$, We have then,

$$dp = c_w^2 \, d\rho + \alpha \, d\eta + \beta_1 \, ds_1 + \beta_2 \, ds_2, \tag{6.78}$$

c_w is the Wood speed of sound defined from the following derivative of the state law of the mixture $p = P(\rho, \eta, s_1, s_1)$:

$$c_w^2 = \frac{\partial P}{\partial \rho}\Big)_{s_1, s_2, \eta}, \tag{6.79}$$

$$\frac{1}{\rho^2 c_w^2} = \frac{\eta}{(\rho_1)^2 (c_1)^2} + \frac{1-\eta}{(\rho_2)^2 (c_2)^2}\,. \tag{6.80}$$

To study waves behaviors we do not need to specify the expressions of the coefficients α, β_1 and β_2. Adding viscosity effect, The linearized rzDFM system in one-dimensional around a constant solution $(\rho_0, u, \eta_0, s_1^0, s_2^0)$ is given by

$$\partial_t \rho = -u_0 \partial_x \rho - \rho \partial_x u\,, \tag{6.81}$$

$$\partial_t u = -u_0\, \partial_x u - \frac{c_w^2}{\rho_0}\partial_x \rho - \frac{\alpha}{\rho_0}\partial_x \eta - \frac{\beta_1}{\rho_0}\partial_x s_1 - \frac{\beta_2}{\rho_0}\partial_x s_2 + \frac{\alpha_1\mu_1 + \alpha_2\mu_2}{\rho_0}\,\partial_{xx}^2 u\,, \tag{6.82}$$

$$\partial_t \eta = -u_0\, \partial_x \eta\,, \tag{6.83}$$

$$\partial_t s_k = -u_0\, \partial_x s_k\,. \tag{6.84}$$

We seek a plane wave solution of the form $U_0 \exp(i\omega\, t + kx)$. We get then

$$\left[i\omega I + kA - k^2 B\right] U = F. \tag{6.85}$$

where

$$A = \begin{bmatrix} 0 & 0 & \frac{\alpha_1 c_1^2 c_2^2 \rho_1 \rho_2 + \alpha_2 c_1^2 c_2^2 \rho_1 \rho_2}{\alpha_1 c_2^2 \rho_2 + \alpha_2 c_1^2 \rho_1} \\ 0 & 0 & \frac{\alpha_1 \alpha_2 c_1^2 \rho_1 - \alpha_1 \alpha_2 c_2^2 \rho_2}{\alpha_1 c_2^2 \rho_2 + \alpha_2 c_1^2 \rho_1} \\ \frac{1}{\rho} & 0 & 0 \end{bmatrix}, B = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\alpha_1 \mu_1 + \alpha_2 \mu_2}{\rho} \end{bmatrix}$$

To simplify we take $u_0 = 0$ which means that the mixture is stagnant. Then non-zero solutions exists if the frequency ω and the complex wavelength verify the following bi-quadratic polynomial on k :

$$c_w^2 k^2 \rho + i k^2 \mu \omega + \omega^2 \rho = 0,$$

Where $\mu = \alpha_1 \mu_1 + \alpha_2 \mu_2$. For a wave of frequency ω such as $K_n = \frac{\mu \omega}{\rho c_w^2} \ll 1$, And thus the dispersion relations and the attenuation coefficient is given by the following formulas [Benjelloun and Zaidni, 2021]:

$$d(\omega) \approx c_w \left(1 + \frac{3\mu^2 \omega^2}{8\rho^2 c_w^4}\right), \qquad a(\omega) \approx -\frac{\mu \omega^2}{2\rho\, c_w^3}.$$

Remark 3. *In the case of zDFM, the Wood speed (6.80) is equal to the speed of propagation (6.64)* $c_\infty = \frac{\omega}{k}(\mu_1 = \mu_2 = 0) = c_w$. *Which is not the case in TVM. So considering signl-pressure* ($p_1 = p_2$) *and suppose that the particles of the mixture have different orbits* ($q_1 \neq q_2$) *imply that* $c_w \neq c_\infty$. *Let's compare the speeds,*

$$\frac{c_w^2}{c_\infty^2} = \frac{1}{(\alpha_1 \rho_2 + \alpha_2 \rho_1)\left(\frac{\alpha_1}{\rho_2} + \frac{\alpha_2}{\rho_1}\right)} \tag{6.86}$$

Lemma 5. *Generalized mean inequality [Bullen, 2013]*

Let p and q two non-zero real numbers, such that $p < q$, and $\lambda_1, \ldots, \lambda_n \in \mathbb{R}_0^+$ with, $\lambda_1 + \ldots + \lambda_n = 1$, then for all strictly positive real $a_1, \ldots, a_n$, we have:

$$\left(\sum_{i=1}^{n} \lambda_i a_i^p\right)^{1/p} \leq \left(\sum_{i=1}^{n} \lambda_i a_i^q\right)^{1/q} \tag{6.87}$$

The equality occurs if and only if $a_1 = a_2 = \ldots = a_n$.

Using the lemma 5 with taking $n = 2$, $p = -1$, $q = 1$, $\lambda_1 = \alpha_1$, $\lambda_2 = \alpha_2$, $a_1 = \rho_2$, and $a_2 = \rho_1$, we get:

$$\frac{1}{\left(\frac{\alpha_1}{\rho_2} + \frac{\alpha_2}{\rho_1}\right)} \leq \alpha_1 \rho_2 + \alpha_2 \rho_1$$

Then we deduce that the Wood speed is lower than the speed of propagation (Phase Velocity),

$$c_w \leq c_\infty \tag{6.88}$$

The equality occurs ($c_\infty = c_w$) if and only if the phases have the same densities $\rho_1 = \rho_2$.

A wave study of the linear mixed hyperbolic-parabolic system of (6.81), (6.82), (6.83), *and* (6.84), *gives the following:*

$$\partial_t U + A\partial_x U = B\partial_{xx} U\,, \tag{6.89}$$

where $U = (u, \rho, \eta, s_1, s_2)$ and the constant matrices A and B given by

$$A = \begin{bmatrix} u & c_w^2/\rho & \alpha/\rho & \beta_1/\rho & \beta_2/\rho \\ \rho & u & 0 & 0 & 0 \\ 0 & 0 & u & 0 & 0 \\ 0 & 0 & 0 & u & 0 \\ 0 & 0 & 0 & 0 & u \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} (\alpha_1\mu_1 + \alpha_2\mu_2)/\rho & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The system (6.89) *with a given initial data, admits a strong solution. This result is a direct application of the fundamental theorems presented in [Kreiss and Lorenz, 2004, see page 166]. In fact writing*

$$B = \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix} \qquad \text{and} \qquad A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix},$$

where

$$B_1 = \left(\frac{\alpha_1\mu_1 + \alpha_2\mu_2}{\rho}\right),\ A_{11} = u,\ A_{12} = \begin{bmatrix} \frac{c_w^2}{\rho} & \frac{\alpha}{\rho} & \frac{\beta}{\rho} \end{bmatrix},\ A_{22} = \begin{bmatrix} u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & u \end{bmatrix}$$

the following conditions are satisfied:

$$B_1 + B_1^* = 2\frac{\alpha_1\mu_1 + \alpha_2\mu_2}{\rho} > 0 \ \textit{and} \quad A_{22} = A_{22}^*.$$

This shows that in the one-dimensional case, the strong solution of the RzDFM exists. Also for the zDFM ($B = 0$), The system (6.89) becomes strictly hyperbolic

and has the symmetrizer:

$$H = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & h & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

where, $h = c_w^2/\rho^2$*, and* $HA = A^*H$*. Thus, the existence of strong solution of nonlinear PDE system of Ideal Drift Flux Model in one-dimensional is proven [Kreiss and Lorenz, 2004, see page 114].*

6.4 CONCLUSION

It has been shown in this chapter that the speed of sound propagation under a single pressure assumption depends on the chosen model. The zDFM yields the classical Wood speed, while the TVM produces a different speed, $c_\infty \neq c_{wood}$, with both speeds coinciding only when the two phases have equal densities. A similar paradox is discussed in remark 1. This indicates that the ill-posedness of the model not only leads to mathematical challenges—such as issues with the existence of solutions, stability, or numerical simulation—but also results in physically questionable outcomes.

CHAPTER

APPENDIX: FUNCTIONAL CALCULUS A

A functional is a map that takes functions into real numbers. To describe a functional properly, we need to define the set of functions it can act on (called a function space) and the rule used to compute the result.

$$\mathcal{B} \longrightarrow \mathbb{R}$$

Just like regular functions, functionals can be continuous, differentiable, and follow rules like the chain rule.

Example: Kinetic Energy of a Fluid

Consider a one-dimensional fluid of constant density. The kinetic energy is given by:

$$T[u] = \frac{1}{2} \int_{x_0}^{x_1} \rho_0 u^2(x)\, dx$$

Here, $u(x)$ is the fluid velocity, and ρ_0 is constant. Given any function $u(x)$, evaluating the integral gives a number.

First Variation and Functional Derivative

If we change $u(x)$ slightly to $u(x) + \epsilon\delta u(x)$, the first variation of a general functional $K[u]$ is:

$$\delta K[u;\delta u] = \frac{d}{d\epsilon} K[u+\epsilon\delta u]\bigg|_{\epsilon=0}$$

If this derivative exists, we can write:

$$\delta K[u;\delta u] = \int_{x_0}^{x_1} \delta u(x)\, \frac{\delta K}{\delta u(x)}\, dx = \left\langle \frac{\delta K}{\delta u}, \delta u \right\rangle$$

The term $\frac{\delta K}{\delta u(x)}$ is called the **functional derivative** of K. The variation is linear in δu, but not necessarily in u. For the kinetic energy functional

$$T[u] = \frac{1}{2}\int_{x_0}^{x_1} \rho_0 u^2(x)\, dx,$$

the first variation is

$$\delta T[u;\delta u] = \int_{x_0}^{x_1} \rho_0 u(x)\delta u(x)\, dx,$$

and thus the functional derivative is:

$$\frac{\delta T}{\delta u} = \rho_0 u.$$

This is similar to the gradient of a multivariable function:

$$df(x;dx) = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} dx_i = \nabla f \cdot dx.$$

General Functional with Derivatives

Let

$$F[u] = \int_{x_0}^{x_1} F(x, u, u_x, u_{xx}, \dots)\, dx.$$

Then

$$\delta F[u;\delta u] = \int_{x_0}^{x_1} \left(\frac{\partial F}{\partial u}\delta u + \frac{\partial F}{\partial u_x}\delta u_x + \frac{\partial F}{\partial u_{xx}}\delta u_{xx} + \cdots \right) dx.$$

Integrating by parts and dropping boundary terms:

$$\delta F[u;\delta u] = \int_{x_0}^{x_1} \delta u(x) \left(\frac{\partial F}{\partial u} - \frac{d}{dx}\frac{\partial F}{\partial u_x} + \frac{d^2}{dx^2}\frac{\partial F}{\partial u_{xx}} - \cdots \right) dx.$$

Thus, the functional derivative is:

$$\frac{\delta F}{\delta u} = \frac{\partial F}{\partial u} - \frac{d}{dx}\frac{\partial F}{\partial u_x} + \frac{d^2}{dx^2}\frac{\partial F}{\partial u_{xx}} - \cdots .$$

Dirac Delta Identity

A useful identity in functional calculus is:

$$u(y) = \int \delta(x-y)u(x)\,dx, \quad \text{so that} \quad \frac{\delta u(y)}{\delta u(x)} = \delta(x-y).$$

CHAPTER

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