What is Variational Thermodynamics?

François Gay-Balmaz*

Critical Action Principles. One of the most fundamental principles in physics is the Principle of Critical Action. Maxwell's equations in electromagnetism, Newton's equations of motion in classical mechanics, Schrödinger's equations in quantum mechanics, and Einstein's equations in general relativity can all be obtained by extremizing a quantity, called action functional, which encodes the properties of the system. The simplest incarnation of this principle is Hamilton's principle in Lagrangian mechanics:

$$\delta \int_0^T L(q, \dot{q}) \mathrm{d}t = 0, \tag{1}$$

which asserts that the actual trajectory of a system is the one that makes the time integral of the Lagrangian critical among possible trajectories. Beyond their historical significance, Critical Action Principles continue to play a fundamental role in modeling physical theories today, serving both applied and theoretical purposes, and offering a unifying approach across multidisciplinary developments.

Towards a Variational Formulation in Macroscopic Nonequilibrium Thermodynamics. The goal of Variational Thermodynamics is to develop variational principles that consistently extend the classical Critical Action Principles of physical theories to include irreversible processes within the framework of Nonequilibrium Thermodynamics in its macroscopic description ([19, 29, 31, 23, 22, 24]). It is important to note that, due to its phenomenological nature and its relevance across a wide range of disciplines, Nonequilibrium Thermodynamics has been developed from various perspectives and techniques. These developments are often closely tied to their specific fields, often resulting in disconnections between them and making it challenging to transpose concepts across different areas. The goal of Variational Thermodynamics is to provide a unifying framework, akin to the Critical Action Principles mentioned earlier, that can encompass a broad range of Nonequilibrium Thermodynamic systems in their macroscopic descriptions. We emphasize that the goal so far only concerns macroscopic descriptions, with the intention of bridging the gap between theoretical formulations and practical applications.

Variational Principles and Thermodynamics. Several variational approaches have been proposed in relation with Thermodynamics. At the heart of most of these is the *principle of least dissipation of energy*, as introduced in [25] and later extended in [26] and [27], which underlies the reciprocal relations in the linear case. Another principle was formulated by [28], [18] as a condition on steady state processes, known as the *principle of minimum entropy production*. Onsager's approach was generalized in [32] to the case of systems with nonlinear phenomenological laws. We refer to [20] for reviews and developments of Onsager's variational principles, as well as for a study of the relationship between Onsager's and Prigogine's principles. In this direction, we also refer to e.g. [23, §6] and [21] for overviews on variational approaches to irreversible processes. Unlike Variational Thermodynamics, these principles do not seek to extend the Critical Action Principles alluded earlier, such as (1). Rather than capturing the complete evolution of a system, they primarily

*School of Physical and Mathematical Science, Nanyang Technological University, francois.gb@ntu.edu.sg

focus on the entropy production equation, aiming to derive the phenomenological laws governing the irreversible processes involved. We refer to [30] and the references therein for a discussion on the construction of variational principles underlying the differential equations of physical theories.

Statement of Variational Thermodynamics. Consider a (possibly open) thermodynamic system subject to internal irreversible processes, labeled α, and irreversible processes at the ports, labeled β. The corresponding thermodynamics fluxes are J_α and J_β, the thermodynamic forces are X^α and X^β, and the thermodynamic forces associated with the exterior are X^β_{ext}. In its current development, as outlined in [14, 15, 16, 17], Variational Thermodynamics takes the following form. First, the thermodynamic displacements Λ^α, Λ^β are defined such that $\dot{\Lambda}^\alpha = X^\alpha$ and $\dot{\Lambda}^\beta = X^\beta$. Then, given the total Lagrangian L of the system, Hamilton's principle (1) is extended in the following d'Alembert form

$$\delta \int_0^T L \, \mathrm{d}t = 0 \quad \text{with} \quad \begin{cases} \dfrac{\partial L}{\partial S}\dot{\Sigma} = J_\alpha \dot{\Lambda}^\alpha + J_\beta(\dot{\Lambda}^\beta - X^\beta_{\text{ext}}) \\ \dfrac{\partial L}{\partial S}\delta\Sigma = J_\alpha \delta\Lambda^\alpha + J_\beta \delta\Lambda^\beta, \end{cases} \tag{2}$$

with $\dot{\Sigma}$ the rate of internal entropy production. The second line on the right describes the constraint to be used on the variations of the variables when computing the critical curve of the action integral. The form of this constraint directly follows by replacing the actual time rate of change in the first line with its virtual form, following d'Alembert's treatment.

Application of Variational Thermodynamics. The principle (2) applies in both finite and infinite-dimensional (i.e., continuum) contexts. Typical applications of this principle include thermomechanical systems, heat exchangers, chemical reaction dynamics, membrane transfer, and heat conducting viscous fluids ([14, 15, 16, 17]). On one hand, Variational Thermodynamics provides a unified method to recover several previously derived models across different fields. On the other hand, it offers an essential approach for deriving thermodynamically consistent dynamical models, particularly in situations where more traditional methods may become intricate or inapplicable. For instance, see [12, 7] for applications in oceanic and atmospheric thermodynamics, [13] for porous media, and [8, 9, 10, 5] for general relativity and cosmology. Additionally, it serves as a fundamental framework for developing thermodynamically consistent numerical methods, see [11] for heat conducting viscous fluids, with many developments still to come.

Connections with Information Geometry. While there is a significant link between Information Geometry and Nonequilibrium Thermodynamics ([2, 1, 6]), it is currently not known how to relate the optimization principles of Information Geometry to the macroscopic variational formulation used in Variational Thermodynamics. Further investigation into such relations is underway for specific classes of thermodynamic systems, aiming to exploit the geometric concepts of Information Geometry alongside the laws of thermodynamics. This exploration could reveal insights into the underlying variational structures that govern thermodynamic processes and their information-theoretic interpretations. Future work may extend these principles to microscopic levels, where statistical mechanics and fluctuations play a critical role, thus improving our understanding of nonequilibrium phenomena across different scales and contexts, beyond what is captured by the current status (2) of Variational Thermodynamics.

References

[1] Amari, S. [2016], *Information geometry and its applications*, volume 194. Springer.

[2] Amari, S. and H. Nagaoka [2000], Methods of Information Geometry (Oxford University Press, 2000) (Originally published in Japanese by Iwanami Shoten, Tokyo, Japan, 1993)

[3] Biot, M. A. [1975], A virtual dissipation principle and Lagrangian equations in non-linear irreversible thermodynamics, *Acad. Roy. Belg. Bull. Cl. Sci.* **5** (61), 6–30.

[4] Biot, M. A. [1984], New variational-Lagrangian irreversible thermodynamics with application to viscous flow, reaction-diffusion, and solid mechanics. *Adv. Appl. Mech.* **24**, 1–91.

[5] Chakrabarti, S. [2024], Phase transition and thermodynamic stability in an entropy-driven universe, arXiv preprint arXiv:2403.12622, 2024.

[6] Cover, T. M. and J. A. Thomas [1991], *Elements of Information Theory*, Wiley: New York, NY, USA.

[7] Eldred, C. and F. Gay-Balmaz [2021], Thermodynamically consistent semi-compressible fluids: a variational perspective, *Journal of Physics A: Mathematical and Theoretical*, **54**, 345701.

[8] Espinosa-Portalés [2022], *Quantum and Thermodynamic Windows into the Universe*, PhD thesis, Universidad Autónoma de Madrid.

[9] Espinosa-Portalés, L. and J. García-Bellido [2021], Covariant formulation of non-equilibrium thermodynamics in General Relativity, *Physics of the Dark Universe*, **34**, 100893.

[10] Espinosa-Portalés, L. and J. García-Bellido [2023], Entropy and irreversible processes in gravity and cosmology. In *The Sixteenth Marcel Grossmann Meeting* (pp. 2013–2028). World Scientific. 5-10 July 2021.

[11] Gawlik, E. S. and F. Gay-Balmaz [2024], Variational and thermodynamically consistent finite element discretization for heat conducting viscous fluids, *Mathematical Models and Methods in Applied Sciences*, **34**(2), 243–284.

[12] Gay-Balmaz, F. [2019], A variational derivation of the nonequilibrium thermodynamics of a moist atmosphere with rain process and its pseudoincompressible approximation, *Geophysical & Astrophysical Fluid Dynamics*, **113**:5-6, 428–465.

[13] Gay-Balmaz, F. and V. Putkaradze [2022], Variational geometric approach to the thermodynamics of porous media, *Zeitschrift für Angewandte Mathematik und Mechanik*, **102**(11).

[14] Gay-Balmaz, F. and H. Yoshimura [2017], A Lagrangian variational formulation for nonequilibrium thermodynamics. Part I: discrete systems, *J. Geom. Phys.*, **111**, 169–193.

[15] Gay-Balmaz, F. and H. Yoshimura [2017], A Lagrangian variational formulation for nonequilibrium thermodynamics. Part II: continuum, *J. Geom. Phys.*, **111**, 194–212.

[16] Gay-Balmaz, F. and H. Yoshimura [2018], A variational formulation of nonequilibrium thermodynamics for discrete open systems with mass and heat transfer, *Entropy*, **20**(3), 163.

[17] Gay-Balmaz, F. and H. Yoshimura [2019], From Lagrangian mechanics to nonequilibrium thermodynamics: a variational perspective, *Entropy*, **21**(1), 8.

[18] Glansdorff, P. and I. Prigogine [1971], *Thermodynamic Theory of Structure, Stability, and Fluctuations*, Wiley-Interscience.

[19] de Groot, S. R and P. Mazur [1969], *Nonequilibrium Thermodynamics*, North-Holland.

[20] Gyarmati, I. [1970], *Nonequilibrium Thermodynamics: Field Theory and Variational Principles*, Springer-Verlag, New York.

[21] Ichiyanagi M. [1994], Variational principles in irreversible processes, *Phys. Rep.* **243**, 125–182.

[22] Kondepudi, D. and I. Prigogine [1998], *Modern Thermodynamics*, John Wiley & Sons.

[23] Lavenda, B. H. [1978], *Thermodynamics of Irreversible Processes*, Macmillan, London.

[24] Lebon, G., D. Jou, and J. Casas-Vásquez [2008], *Understanding Non-equilibrium Thermodynamics*, Springer-Verlag Berlin Heidelberg

[25] Onsager, L. [1931], Reciprocal relations in irreversible processes I, *Phys. Rev.* **37**, 405–426; Reciprocal relations in irreversible processes II, *Phys. Rev.* **38**, 2265–2279.

[26] Onsager, L. and S. Machlup [1953], Fluctuations and irreversible processes, *Phys. Rev.* **91**, 1505–1512.

[27] Onsager, L. and S. Machlup [1953], Fluctuations and irreversible processes II. Systems with kinetic energy. *Phys. Rev.* **91**, 1512–1515.

[28] Prigogine [1947], *Etude Thermodynamique des Phénomènes Irréversibles*, Thesis, Paris: Dunod and Liège: Desoer.

[29] Stueckelberg, E. C. G. and P. B. Scheurer [1974], *Thermocinétique Phénoménologique Galiléenne*, Birkhäuser, 1974.

[30] Van, P. and B. Nyiri [1999], Hamilton formalism and variational principle construction, *Ann. Phys. (Leipzig)* **8** 4, 331–354.

[31] Woods, L. C. [1975], *The Thermodynamics of Fluid Systems*, Clarendon Press Oxford 1975.

[32] Ziegler, H. [1968], A possible generalization of Onsager's theory, in H. Barkus and L.I. Sedov (eds.), *Irreversible Aspects of Continuum Mechanics*, Springer, New York.