Entrophy and convexity for nonlinear partial differential equations

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Partial differential equations are ubiquitous in almost all applications of mathematics, where they provide a natural mathematical description of many phenomena involving change in physical, chemical, biological and social processes. The concept of entropy originated in thermodynamics and statistical physics during the nineteenth century to describe the heat exchanges that occur in the thermal processes in a thermodynamic system, while the original notion of convexity is for sets and functions in mathematics. Since then, entropy and convexity have become two of the most important concepts in mathematics. In particular, nonlinear methods via entropy and convexity have been playing an increasingly important role in the analysis of nonlinear partial differential equations in recent decades. This opening article of the Theme Issue is intended to provide an introduction to entropy, convexity and related nonlinear methods for the analysis of nonlinear partial differential equations. We also provide a brief discussion about the content and contributions of the papers that make up this Theme Issue.

1. Introduction

Partial differential equations (PDEs) are ubiquitous in almost all applications of mathematics, where they provide a natural mathematical description of many phenomena involving change in physical, chemical, biological and social processes. The behaviour of every material object, with length scales ranging from subatomic to astronomical and timescales ranging from picoseconds to millennia, can be modelled by PDEs or by equations having similar features. The concept of entropy originated in thermodynamics and statistical physics during the nineteenth century to describe the heat exchanges that occur in the thermal processes in a thermodynamic system, whereas the
original notion of convexity is for sets and functions in mathematics. Since then, entropy and convexity have become two of the most important concepts in mathematics. In particular, nonlinear methods via entropy and convexity have been playing an increasingly important role in the analysis of nonlinear PDEs in recent decades. For example, for discontinuous or singular solutions to nonlinear conservation laws which may contain shock waves and concentrations, the notion of entropy solutions is based on entropy conditions involving convexity, motivated by and consistent with the Second Law of Thermodynamics. In addition, entropy methods have become one of the most efficient methods in the analysis of physically relevant discontinuous or singular solutions. The notions of convexity appropriate for multi-dimensional problems, such as polyconvexity, quasi-convexity and rank-one convexity, are responsible for several recent major advances. In the last three decades, various nonlinear methods involving entropy and convexity have been developed to deal with discontinuous and singular solutions in different areas of PDEs, especially in nonlinear conservation laws, the calculus of variations and gradient flows.

This Theme Issue is devoted to fundamental questions concerning entropy, convexity and related nonlinear methods designed to help to understand the very difficult problems posed by multi-dimensional, nonlinear PDE problems. In particular, it includes the discussion of several recent developments in nonlinear methods via entropy and convexity, the exploration of their underlying connections, and the development of new unifying methods, ideas, and insights involving entropy and convexity for important multi-dimensional PDE problems in fluid/solid mechanics and other areas. These new developments are at the forefront of current research.

2. Entropy

The concept and name of entropy, as a mathematical quantity, originated in the early 1850s in the work of Rudolf Julius Emmanuel Clausius (1822–1888) [1], built on the previous intuition of Nicolas Léonard Sadi Carnot (1796–1832) [2]; Entropy, as an extensive thermodynamic function of state, describes the heat exchanges that occur in thermal processes from the macroscopic point of view. Ludwig Edward Boltzmann (1844–1906) first observed that the Clausius entropy associated with a system in equilibrium is proportional to the logarithm of the number of microstates in microscopic dynamics which form the macrostate of this equilibrium; this exposed a symbiotical relation between the notions of entropy from both macroscopic and microscopic points of view [3]. Similar ideas were also developed by many physicists and mathematicians of those times, most notably James Clerk Maxwell (1831–1879), Josiah Willard Gibbs (1839–1903), Max Karl Ernst Ludwig Planck (1858–1947) as well as Constantin Carathéodory (1873–1950); see [4–7]. There remain many issues concerning the relation between the microscopic and macroscopic descriptions of matter which are not completely resolved, notably concerning the manner in which irreversibility at the macroscopic level is consistent with reversible dynamics at the microscopic level.

A key contribution of Boltzmann (cf. [3]) was to note that the Maxwell–Boltzmann equation of the kinetic theory of gases possesses a Lyapunov function related to entropy, the Boltzmann $H$-function. Macroscopic statements of the Second Law of Thermodynamics, such as the Clausius–Duhem inequality, deliver similar Lyapunov functions for solutions satisfying the balance laws of mass, momentum and energy (see Duhem [8] and Ericksen [9]), which, depending on the boundary conditions, is either the total entropy or the so-called ballistic free energy (when the boundary is in contact with a heat bath maintained at a temperature that is constant in space and time). The situation is more complicated for spatially dependent boundary temperatures; see [10]. The existence of such Lyapunov functions links dynamics to energy minimization, providing a dynamic motivation for the calculus of variations. However, there remains a large theoretical gap between Boltzmann’s $H$-theorem, applying as it does to a moderately rarified gas and macroscopic statements of the Second Law, which are routinely applied to a much wider class of materials.
Since the work of these pioneers, entropy has become one of the most important concepts in the sciences, and various entropy approaches have been developed which have had a considerable impact on many important areas of mathematics and related sciences. These areas include continuum mechanics, kinetic theory, statistical physics, probability, stochastic processes and random fields, dynamical systems and ergodic theory, information and coding, data analysis and statistical inference, in addition to PDEs. Ideas involving entropy have played a crucial role in developing many important mathematical approaches and methods, such as variational principles, Lyapunov functionals, relative entropy methods, monotonicity methods, weak convergence methods, divergence-measure fields and kinetic methods (cf. [11–30]).

Entropy methods for nonlinear PDEs are techniques and approaches for discovering and exploiting dissipation inequalities for nonlinear PDEs. As noted in Evans [25], these approaches reflect the insight that nonlinear PDEs are generally too hard to grapple with directly, and so often a good idea is to simplify by integrating out various expressions involving the solutions to gain more information about them. The advantage of entropy methods is the elegance in their formulation and generality in their applications (cf. [13,14,17,23,24,27,29]).

3. Convexity

The original notion of convexity in mathematics is for sets and functions. In Euclidean space, a set is convex if, for every pair of points within the set, every point on the straight line segment that joins them is also within the set. A real-valued function defined on an interval is said to be convex if the graph of the function does not lie above the line segment joining any two points of the graph. It has been generalized to more significant settings, especially for functionals, which have played an important role in many areas of mathematics, including functional analysis, complex analysis, differential geometry, topology, geometric measure theory, optimization theory, the calculus of variations, in addition to PDEs. Convex analysis has become an important branch of mathematics devoted to the study of properties of convex functions, convex sets and convex functionals, which occur in the analysis of PDEs.

In particular, convexity plays an important role for entropy methods for PDEs, especially for conservation laws, the calculus of variations, gradient flows, among others. For example, for a system of conservation laws, the existence of a strictly convex entropy for the system ensures its hyperbolicity; the relative entropy methods via convexity have proved very useful for establishing the existence, stability and structure of solutions, as well as hydrodynamic limits of large particle systems, for various PDEs. The notions of convexity appropriate for multi-dimensional problems, such as polyconvexity, quasi-convexity and rank-one convexity, have been fundamental in the theory of nonlinear PDEs and the calculus of variations (cf. [15,17,18,24,26,31–33]).

4. Entropy and convexity for nonlinear PDEs and related areas

The topics of this Theme Issue are cross-disciplinary. The following areas are brought together in the issue: hyperbolic conservation laws, elliptic/parabolic equations, the calculus of variations, continuum mechanics, kinetic theory, statistical physics, probability, plasma physics, astrophysics, materials science, dynamical systems, optimal transportation, differential geometry, among others. The underlying connection between them is entropy and convexity.

The paper by Adams et al. [21] provides a survey of recent activities in deriving and explaining macroscopic evolution equations via entropy for multi-particle systems. Heat flows are gradient flows in the space of probability measures, whose microscopic origin can be justified by using the formalism of statistical mechanics. This is done by computing entropy as a rate function via the theory of large deviations and by identifying the variational structures concerning fluctuations around the gradient flow, because the zero entropy path is the most likely path (mean-field), which is the gradient flow; the other possible paths permitted in the microscopic model correspond to fluctuations around such a path with a cost (entropy). The variational
In particular, the emerging potential of a bigger picture is present, namely that entropies and thermodynamic free energies can be derived via large deviation principles, at least for some non-equilibrium situations, and the two concepts of large deviation principles for stochastic particle systems and gradient flows are closely entwined. The approach advocated in [21] is different from the established hydrodynamic limit passage and extends a link that is well known in the equilibrium situation.

Blesgen & Chenchiah in [22] consider the effects of elastic energy (i.e. stress) on the evolution of microstructure formation on smaller length scales, known as coarsening, which are modelled by time-dependent nonlinear PDEs. Coarsening is driven by both the interfacial and elastic energy. The equilibrium state for coarsening driven purely by the interfacial energy is a single spherical inclusion that minimizes the interfacial area. By contrast, the equilibrium state for coarsening driven by the elastic energy alone is mathematically challenging and is a microstructure on an infinitesimal scale. In [22], the key experimental observations pertaining to coarsening in elastic solids are summarized; the Cahn–Larché model, a generalization of the Cahn–Hilliard equation that incorporates a quasi-convex elastic energy density obtained from relaxation, is analysed; some recent developments concerning the two-scale model for elasticity-influenced coarsening are presented, including several motivations, analytical results and comparisons of the model with experimental results; and some further mathematical reflections and questions are addressed.

The paper by Brenier [23] provides deep, somewhat unexpected, connections of convexity and entropy with the mathematical theory of convection through the mathematical concept of rearrangement. Rearrangement theory is about reorganizing a given function or map in some specific order, for example as an increasing function or a map with convex potential. The convection of a fluid leads to fluid parcels being continuously reorganized in a stabler way under the action of the buoyancy force. Convection is one of the most important phenomena in nature with many important applications. The connections are exposed through deep insights into relations between the so-called transport–collapse method to solve conservation laws, some interesting social science models and the structure of some convection models in meteorological sciences. In particular, the theory enlightens the mechanism involved in the hydrostatic limit of the Navier-Stokes–Boussinesq equations. The limit is obtained via a relative entropy method under a natural convexity condition.

Hyperbolic systems of conservation laws are one of the most important classes of nonlinear PDEs. As a consequence of the Second Law of Thermodynamics, systems of conservation laws arising in continuum physics are endowed with an entropy function of the state variable. In many cases, the entropy function is convex, which is the case for the Euler equations for elastic fluids, the prototype of hyperbolic systems of conservation laws. Convexity of the entropy leads to the local well-posedness of the Cauchy problem in a Sobolev space of sufficiently high order, as well as the $L^2$-stability of the solution even within the broader class of entropy solutions (cf. [10,12,16]). However, convexity of the entropy function is not ubiquitous; such examples include important systems of conservation laws in continuum mechanics, thermomechanics and electrodynamics, especially the equations of elastodynamics, for which convexity of the entropy is incompatible with geometric invariance dictated by physics. Quite often, failure of convexity of the entropy function is encountered in systems endowed with involutions. As observed by Dafermos [24], involutions may compensate for the loss of convexity; indeed, under the assumption that the contingent entropy function is convex merely in the direction of the involution cone in state space, it is shown in [24] that the Cauchy problem is still locally well-posed in the class of classical solutions, and that classical solutions are unique and stable even within the broader class of entropy solutions. In the process, technical subtleties that were glossed over in earlier treatments are also presented in detail. The theory is an important
generalization of the classical local well-posedness theory to nonlinear systems of conservation laws equipped with involutions and partially convex entropies, which include many important physical systems.

The paper by Evans [25] concerns monotonicity methods for nonlinear PDEs arising from variational problems. Monotonicity methods and entropy methods are strongly related. For monotonicity formulae, various expressions involving the solution are integrated over a ball $B(x, r)$ of centre $x \in \mathbb{R}^n$ and radius $r$ in the Euclidean space $\mathbb{R}^n$, in order to get useful differential inequalities determining how these integrals depend on the radius $r$. The artistry for this approach (as well as the entropy approach) is in the design of the precise expressions that are integrated. To illustrate the approach, it is shown in [25] how certain explicit integral formulae are derived involving the solutions of elliptic PDEs corresponding to stationary points of functionals having the form

$$\int_{\mathcal{U}} F(Du) \, dx \quad \text{for } u : \mathcal{U} \subset \mathbb{R}^n \to \mathbb{R}^m,$$

where $Du$ is the gradient of $u$. Three important special cases are treated as illustrations: (i) $m = 1$ and $F(p) = |p|_2$; (ii) $m > 1$ and $F(M) = \frac{1}{2} |M|^2$; and (iii) $m = n$ and $F(M) = \frac{1}{2} |M|^2 + 1/(\det M)^{\gamma}$. The approach and ideas presented will stimulate further work in this direction.

Liero & Mielke in [26] analyse systems of parabolic PDEs involving diffusion, drift and reaction. As observed in [26], under natural physical assumptions, these systems have the structure of a gradient flow with respect to an entropy functional and dissipation Riemannian metric given in terms of a so-called Onsager operator, which is a sum of a diffusion part of Wasserstein type and a reaction part. New methods are provided for establishing geodesic $\lambda$-convexity of the entropy functional by purely differential methods, circumventing arguments from mass transportation. Contraction properties of these gradient flows with respect to the intrinsic dissipation metric are analysed. Sufficient conditions for contractivity are derived for several important physical examples including a drift–diffusion system, which provides a survey on the applicability of the theory.

The paper by Liu [27] samples some of recent analytical developments in the study of dissipation around the entropy methods for hyperbolic conservation laws, viscous conservation laws and the Boltzmann equation. As discussed in [27] through different examples, several types of dissipation, such as the viscosity and heat conductivity, the nonlinearity and the coupling of distinct characteristics, occur in both the hyperbolic and viscous systems of conservation laws. In particular, the relationship between kinetic theory and compressible fluid dynamics is explained, and dissipation caused by the intermolecular collisions in kinetic theory is addressed. In addition, the importance of dissipation due to boundary effects is emphasized. The Green function approach, a qualitative way based on concrete constructions, is another useful approach to understand the dissipation and the relation between gas dynamics and kinetic theory. There is much room for future progress for the entropy methods, the Green function approach and other possibilities in this direction.

Penrose in [28] provides a clear illustration of the importance of phase space volume in the definition of entropy and effective irreversible behaviour for chaotic dynamical systems. More precisely, a new non-equilibrium entropy or trajectory entropy for chaotic dynamical systems is proposed, whose main feature is that it does not require any use of the concept of a macroscopic state of the dynamical system. For any given $\varepsilon > 0$ and two phase points lying on the two endpoints of a given trajectory of the system, the so-called dynamical self-correlation of the two endpoints is roughly the conditional probability that, if the system is started at initial time from a phase point chosen uniformly in a ball, then its phase point at the terminal time will lie in an $\varepsilon$-neighbourhood of the original terminal phase point. The proposed entropy is then the logarithm of the inverse of the dynamical self-correlation. The main issue is the conjecture made that the dynamical self-correlation converges in the limit of diverging time (between the chosen phase points of the trajectory) to the quotient of the phase space measure of the $\varepsilon$-ball and the total phase space measure of the given system. Partial support for this conjecture is provided through two examples of dynamical systems. The conjecture allows one to connect the limit of the
self-correlation to the equilibrium entropy, and thus the definition of the new entropy becomes a
natural object to consider, that is, the non-equilibrium entropy is proportional to the logarithm of
the quotient of the phase space measure of the $\varepsilon$-ball and the self-correlation, for the phase points.
The idea is illustrated by using an example based on Arnold’s ‘cat’ map, which also demonstrates
that it is possible to have irreversible behaviour, involving a large increase of entropy, in a chaotic
system with only two degrees of freedom.

Saint-Raymond in [29] discusses Boltzmann’s $H$-theorem and its essential role in rigorous
derivation of fluid dynamics equations from the Boltzmann equation, which justify the
mathematical significance of the notion of entropy. The main focus is on the study of
hydrodynamic limits in the framework of solutions defined by the physical energy and entropy
bounds, at both the kinetic and fluid level. The analogies between several kinetic and fluid
models are detailed by examining the use of the entropy inequality and the implications for
functional analysis. The modulated entropy method and the kinetic formulation approach are
suggested. The hydrodynamic regime which has been best understood is the one that leads
to the incompressible Navier–Stokes equations, which is indeed the only asymptotics of the
Boltzmann equation for which an optimal convergence result is known via the scaled relative
entropy inequality (cf. Golse & Saint-Raymond [19]).

In Slemrod [30], three notions of admissibility for weak solutions are discussed through
the isentropic Euler equations of gas dynamics: the viscosity criterion, the entropy inequality (the
thermodynamically admissible isentropic solutions), and the viscosity–capillarity criterion.
The Chapman–Enskog expansion for the Boltzmann equation, when truncated to orders
beyond the first order (Burnett and super-Burnett approximations), is known to produce
approximations of the compressible Euler equations, for which the equilibrium flow is unstable
or at most conditionally stable. The dominant view is that the problem is not the Chapman–
Enskog expansion but the truncation of the expansion. The focus of this paper is on a simplified
model for a one-dimensional flow of Grad’s linearized 13 moment system. For this system, the
Chapman–Enskog expansion can be exactly summed, and the dispersion relation is calculated
accurately to all orders. The novelty is that the induced entropy inequality is computed, which
has two additional terms: one corresponds to the capillarity contribution to the energy and the
other to the viscous dissipation. Recent results of DeLellis & Szekelyhidi [34] have shown that
the usual concept of entropy solutions is inadequate to imply uniqueness for the incompressible
and the compressible Euler equations. This raises the issue of how this ‘paradox’ is interpreted
or alternatively how the concept of entropy in weak solutions is improved/replaced by an
alternative concept. It is conjectured in [30] that the energy dissipation, obtained when the
compressible Euler equations are viewed from the perspective of kinetic theory, has additional
terms relative to the one obtained when viewed as a limit from the compressible Navier–
Stokes system. This is indeed justified through the simplified model. Further investigations and
explorations are needed to understand the non-uniqueness issue, which is closely related to
entropy and convexity.

5. Outlooks

As we have briefly discussed above, entropy and convexity have played an important role in
the recent developments in the analysis of nonlinear PDEs and related areas. The results in
the papers of this Theme Issue present a deeper understanding of existing nonlinear methods
via entropy and convexity and their underlying connections in different areas of PDEs, and
open up challenging new research problems and interdisciplinary research directions. Further
developments of unifying nonlinear methods and ideas via entropy and convexity will be useful
for solving some longstanding, challenging problems in nonlinear conservation laws, the calculus
of variations and other areas.

In particular, since the seminal work of Jacques Hadamard in the early 1920s concerning
the classification of linear PDEs, the research community in PDEs has been largely partitioned
by the approaches taken to the mathematical analysis of different classes of PDEs (hyperbolic,
parabolic and elliptic). However, advances in mathematical research on PDEs over the last 30 years have been making it increasingly clear that many difficult questions faced by the community are at the boundaries of this classification or, indeed, go beyond this narrow classification. Several important sets of nonlinear PDEs that arise in fluid mechanics, solid mechanics, materials science, conservation laws, the calculus of variations, geometry, among many others, involve PDEs of mixed type (e.g. mixed hyperbolic–elliptic type and mixed hyperbolic–parabolic type). The unification of the mathematical theory for disparate classes of nonlinear PDEs is at the cutting edge of modern mathematical research and has important implications not only for mathematicians, but also for the wider scientific communities who use nonlinear PDEs. Moreover, a particular challenge concerns the understanding of the roles played in multi-dimensional dynamics by convexity conditions, such as quasi-convexity, which are central to the corresponding variational problems for statics. It is our belief that nonlinear methods and ideas via entropy and convexity will also play a fundamental role in the analysis of nonlinear PDEs of mixed type and for solving longstanding and newly emerging fundamental open problems involving such PDEs, which deserve our special attention.

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