Entropy Methods, PDEs, Functional Inequalities, and Applications (14w5109)

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Entropy methods are one of the fundamental tools for the analysis of nonlinear PDEs, the proof of functional inequalities, and for capturing concentration phenomena in probability theory. This workshop has shown that entropy methods and related theories have clearly acquired maturity, and are of great importance for theoretical considerations and in applications. The scientific community behind the entropy method is very active and has a wide spectrum of interests, ranging from mathematical biology to differential geometry, and from discrete stochastic models and scientific computing, with very diverse motivations at least as far as applications are concerned. The involved researchers share a common knowledge and understand each other well. Workshops at Banff are perfect for extended interactions under such circumstances.

1 Recent Developments, Presentation Highlights and Open Problems

1.1 Advances in the theory

1.1.1 Novel variational approaches

Gradient flows in space of probability measures have provided a powerful tool for establishing well-posedness of a class of dissipative equations, as detailed in the book of Ambrosio, Gigli and Savaré [4]. This meeting has shown that a remarkably broad progress has been made during the last four years on problems and techniques that go beyond the reach of the previously studied setting.

LIERO and SAVARE discussed a new metric on the space of probability measures: the Hellinger-Kantorovich distance. An essential motivation for introducing this metric was to overcome a conceptual limitation of the Wasserstein distance, namely that any two measures of different total mass are infinitely far apart from each other. Instead, the Hellinger-Kantorovich distance allows to compare non-negative measures of arbitrary finite mass. The basic idea is to minimize over "paths" connecting the two measures which involve not only transport, but also annihilation and creation of mass. A key observation about the Hellinger-Kantorovich distance is the following: If measures of compact support are spatially close to each other, then the geodesic between the two is essentially defined by the usual Wasserstein mass transport, only that mass can decrease or grow along the path. If instead the measures are sufficiently far apart in space, then the geodesic path almost exclusively works by teleportation, i.e., annihilation of mass at the source and creation of mass at the target location.

Even though the definition of this metric is very recent, a lot of interesting properties have been proven already, some of them with an intriguing geometric interpretation. Despite the theory being so young and still under strong development, it seems very likely that in the near future, it might play a role in the analysis of reaction–diffusion equations that is comparable to the role that the Wasserstein distance nowadays plays in the context of non-linear diffusion and non-local aggregation equations.

STEFANELLI discussed a general framework for obtaining various nonlinear evolution equations through a convex minimization [2, 25, 27]. The WIDE (Weighted Inertia-Dissipation-Energy) Principle provides a scheme that works well in a significant number of existence problems corresponding to classical evolution equations. A reinterpretion evolution equations in the language of thermodynamics was discussed by ZIMMER. He addressed the question of deriving macroscopic evolutions driven by entropy or free energy from particle models. A dynamic scale-bridging approach based on particle evolutions with noise and the large deviation principle [1, 21] has been developed and applied to a number of problems. In particular it allows to consider the Vlasov-Fokker-Planck equation as GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) equation. This is a promising avenue to formulating such equations and for giving them a structure that merits further exploration. LEONARD discussed the entropy approach to special solutions to the Navier-Stokes equation with fixed initial and final data. This comes as an significant extension of Arnold's approach of the Euler equation. The current task is to understand what is the special status of these solutions among all other ones. KIM [3] talked about approximating solutions of solutions to (nonlinear) parabolic equations on bounded domain with oblique boundary conditions by solutions of equations on the whole space where a drift term has been added outside the original domain. TUDORASCU presented a global existence result for one-dimensional pressureless Euler/Euler-Poisson systems with or without viscosity [28]. It is obtained by employing the sticky particles model. Stability and uniqueness of solutions were obtained via a contraction principle in the Wasserstein metric. WU discussed the gradient flow approach to nonlocal-interaction equations in heterogeneous environments [32]. The fact that mobility varies in space endows the physical space with a manifold structure. Wu studied gradient flows of nonlocal interaction energy on manifolds with boundary including the case of non-convex sets [13].

1.2 Functional inequalities and asymptotic behavior

Entropy methods provide a direct connection between functional inequalities and quantitative estimates of asymptotic behavior of solutions of evolution equations. In typical settings, such as for Fokker-Planck or porous medium equations the functional inequalities provide a quantitative measure of the convexity of the entropy (or free energy) near the equilibrium, which in turn implies rates of convergence of solutions towards the equilibrium. The advances presented go beyond this framework and include equations where uniform convexity of the entropy near the equilibrium does not hold, estimates on asymptotics of discrete approximations, duality based approaches, symmetry breaking and systems of equations.

When participants were asked about their favorite talks by the organizers, several mentioned the presentation of ARNOLD, and said that it gave them an interesting new perspective on one of the oldest topics in entropy methods, namely to estimate the exponential rate of convergence to equilibrium for linear Fokker-Planck equations. The new ingredients for the old problem are hypocoercivity (degeneracy of the diffusion matrix) and non-symmetry (allowing drift terms that are not in gradient form). Both new effects need to be combined in the appropriate way in order to end up with a system whose solutions converge exponentially fast towards a stationary state that is non-degenerate in the sense that it possesses a density function. The talk was restricted to the situation where the drift force is a linear function on space, and it will require significant work to extend the results further. In this linear setting, however, a quite complete characterization of possible combinations of hypercoercive diffusion operators and non-symmetric drifts was given. Old results by Hörmander and more recent results by Villani were combined with genuinely new ideas. In the end, the calculation of the optimal exponential rate of equilibration was reduced to solving surprisingly simple problems in linear algebra.

A quite beautiful geometric approach to functional inequalities was presented by STURM. In his talk, he discussed the role of the auxiliary dimension N in the curvature-dimension condition $CD(K, N)$ for metric measure spaces [5, 14]. In fact, most of the results in the literature on logarithmic Sobolev and transportation inequalities or on the contractivity of the heat flow are concerned with the case in which the dimension parameter is irrelevant, that is $N = \infty$. However, if it is known that a manifold satisfies $CD(K, N)$ with some finite N, then these characteristic inequalities and contraction estimates can be improved both qualitatively and quantitatively. After giving a geometric interpretation of the refined curvature dimension condition, two approaches to the derivation of the improved inequalities were presented: the first is based on a refined analysis of mass transportation on manifolds, the second approach uses the Γ-calculus from the Bakry-Emery method.

FILBET explained that when writing discrete functional inequalities corresponding to a discretization of the continuous problem, the geometry of the mesh enters in the value of the optimal constants. Consequently, numerical rates of convergence towards equilibrium may be faster than expected. Relating best constants in the functional inequalities with discretized evolution equations is a challenging open question.

CAÑIZO discussed the entropy – entropy production inequalities for the linear Boltzman equation [9]. HUANG discussed an application of entropy methods to asymptotic behavior of the porous medium equations with fractional pressure in one dimension. Connection to Bakry-Emery method and transport inequalities was also included. JANKOWIAK discussed the flow which paves the way to further studies mixing gradient flows and duality notions [19]. NAZARET discussed symmetry breaking issues in weighted functional inequalities, which are a severe obstruction for understanding the optimality cases and the asymptotic regimes in the corresponding evolution equations. Moreover, weights raise a number of conceptual difficulties that should be treated with powerful tools like the $CD(\rho, N)$ condition, which turns out to be difficult to implement in practical cases. STAŃCZY talked about a model of gravitating particles [20, 31] that takes the form of a nonlocal parabolic equation. He focused on existence of stationary solutions and showed that for a fixed mass there can exist more than one stationary solution.

1.3 Applications

The range of applicability of the entropy method has been constantly widened in the last decade. In the beginning, applications were centered around the classical topics from mathematical physics, like nonlinear diffusion, or lubrication theory. Then, in the context of the very successful analysis of the Keller-Segel model by entropy methods, applications to systems in biology became very popular, a trend that peaked around the time of the previous entropy workshop at Banff about four years ago. Clearly, macroscopic equations for swarming, herding etc. are an extremely active field of research for the entropy community. The current meeting gave the organizers the impression that reaction-diffusion systems from chemistry might play the pivotal role for applications of the entropy methods in the near future.

This development reflects the successful extension of entropy related concepts to more and more complex equations. First results were concerned with scalar drift-diffusion equations — first linear, then non-linear, possibly degenerate. Later, the entropy structure in fourth (and higher) order non-linear diffusion equations was understood. The biological applications emerged when the theoretical results were extended to equations with non-local interaction terms. In that context, the entropy method was also applied to special systems of two coupled non-linear equations. Current developments aim at gaining a sound understanding of entropy dissipation in much more general systems of coupled diffusion equations. The main difficulty in this most recent step is the complete loss of comparison principles, which poses a more significant problem than it did, e.g., for fourth order diffusion equations.

1.3.1 Reaction-diffusion equations

Mainly due to the absence of comparison principles, reaction-diffusion systems are out of the reach of the standard parabolic theory. The difficulties are not just a short-coming of the techniques: there are rather harmless-looking systems with very few species which admit solutions that blow up in finite time. The talks focussed on systems to which the duality method can be applied, and which consequently do not blow up.

DESVILLETTES and FELLNER discussed progresses made in the theory of systems of reaction-diffusion equations [11], which allows to consider, for instance, networks of linear reversible equations. Purely algebraic computations provide Lyapunov functionals. Lyapunov estimates and duality methods respectively give compactness and prevent concentration. For systems, so far, no Maximum Principle approach can be expected to work. Hence the approach based on the combination of Lyapunov and duality methods is at the moment the only one that provides some hope for a general theory, which is still to be done. GENTIL discussed an interesting result under very special conditions on the coefficients of the system, [23]. The participants were intrigued by the possibility to combine the approach with the techniques discussed by other speakers (Desvillettes and Fellner).

A different point of view on the mathematical modeling of chemical reactions was presented by MAAS. Quite general reactions between K different species were considered, and a time-dependent stochastic model was written down for the number of particles from each of the species. The stochastic dynamics for the corresponding probability densities on $\mathbb{N}^K$ can be formulated as a gradient flow for the relative entropy functional in a suitable transportation metric on the discrete space. Such gradient flows on discrete spaces have recently been advanced by Maas and collaborators [26, 22] The thermodynamic limit (volume going to infinity, keeping the particle densities fixed, so that accordingly $\mathbb{N}^K$ approaches $\mathbb{R}_+^K$) was then rigorously analyzed in the framework of Γ-convergence. The limiting dynamics is governed by a non-linear second order diffusion equation for probability densities $\mathbb{R}_+^K$ (not on physical space), which still has the form of a gradient flow. Clearly, it would be nice to eventually connect these spatially homogeneous dynamics with a clear variational structure to the dynamics for space-dependent concentrations discussed before.

In this context, we further mention again the talks of LIERO and SAVARE, which highlighted a significant advance in the representation of systems with reactions (annihilation and creation of mass) as gradient flows. Currently, this approach is restricted to scalar equations. We expect that the connection between the entropy/duality approach for genuine systems and the novel gradient flow structure will become a key topic for future research.

1.3.2 Biological systems

The thorough analysis of the Keller-Segel system from chemotaxis modelling in the past years is probably one of the greatest success stories for the entropy method. In this workshop, we have had a variety of talks that were concerned with further extensions both of the related analytical tools and of the biological model underlying the equations.

BLANCHET presented a conceptually novel proof for global well-posedness of the parabolic-parabolic Keller-Segel system in the regime of sub-critical mass. The proof is obtained by further development of techniques from an earlier work on the parabolic-elliptic system. The key idea is to write the coupled equations as a gradient flow — in a joint Wasserstein-L^2-metric — of one functional, and to use the dissipation of another Lyapunov functional to derive additional estimates. The general concept of representing systems of evolution equations as gradient flow of *one* functional in a *combined* metric for the components seems promising for a variety of further applications. In fact, novel estimates on the large-time behavior of solutions seem within reach.

The topic of CHEN's talk was the behavior of solutions to (parabolic-elliptic) Keller-Segel systems with non-linear diffusion of power type for the bacterial density [15]. These chemotaxis equations were considered in arbitrary space dimension, and two dimension-dependent critical exponents for the diffusion were defined: the larger one is such that the equations are invariant under mass rescaling, the smaller one is such that the associated entropy functional is conformally invariant. The main result concerns the range of exponents strictly between the critical numbers. Similarly as for the "standard" Keller-Segel system in two dimensions, there is a sharp threshold for an L^p-norm of the initial datum below which the corresponding solution exists globally, and above which it blows up in finite time. The proof combines the standard entropy approach (involving the log-HLS inequality) with suitabel interpolation estimates, and is yet another nice example for the strength of the entropy method.

A different approach to the mathematical modeling of the underlying biological system was discussed by STEVENS. Instead of describing the motion of bacteria by means of a drift towards higher concentrations of the signaling substance which diffuses on a very short time scale, it seems (at least for certain populations of microorganisms) more reasonable to model the motion in terms of reinforced random walks. The resulting "macroscopic" equations have some resemblance to the established Keller-Segel system, but the elliptic equation for the concentration of the signaling substance is replaced by an ordinary differential equation in time. A variety of analytical results has been proven recently about the (non-)existence of global solutions to this kind of systems. The picture is not yet as complete as (and quite different from) the one for the classical Keller-Segel equations, but it seems that the behavior is at least as rich: for all the physically relevant dimensions, parameter regimes for global existence, finite-time blow-up and infinite-time blow-up of solutions have been identified. So far, these results have been obtained mainly by PDE techniques. It will be a challenge for the community to try to recover and hopefully improve them with entropy methods.

A new ansatz for mathematical modeling of a biological system was also the topic SCHMEISER's presentation. Here, the subject was not related to chemotaxis, but to cell motion by flat protrusions (lamellipodia) [29, 30]. The talk visualized the entire route from the very first microscopic modeling ansatz, motivated by observations of biologists in recent experiments, to the analysis of the macroscopic equations by means of the entropy method. It was quite impressive to see how a model developed on a basis of very few (biologically well-supported) assumptions leads to equations with an interesting mathematical structure, and how closely the results on numerical experiments are to the experimental observations. This is a part of long term program of Schmeiser's group on theoretical and numerical approaches for the modeling of the cytoskeleton (actin filaments), a program that will probably provide a number of further structurally interesting equations.

1.3.3 Many-agent systems: patterns and new models

Schools of fish, flocks of birds, and swarms of locust provide widely known examples of organization in many-agent systems. It is believed that the agents in such systems are governed by simple rules which includes the influence of the environment and the interactions with other agents. The nonlocal-interaction equations provide one of the simplest models of such interactions. In addition to them the participants talked about more refined models with an additional function which describes the (emotional) state of the agent, and systems in which agents are "rational" and have well defined goals.

BERTOZZI talked about an agent-based model of emotional contagion coupled with motion in one dimension, [8]. The model involves movement with a speed proportional to a fear variable that undergoes a temporal consensus averaging based on distance to other agents. They studied the Riemann initial data for this problem, leading to shock dynamics that is studied both within the agent-based model as well as in a continuum limit.

CARRILLO and LAURENT talked about patterns arising in models of collective behavior of autonomous agents, more precisely about (local) minimizers of nonlocal-interaction energies. Despite of their simplicity, these exhibit a broad variety of patterns. Laurent presented conditions on the regularity of the interaction potential at the origin that provide estimates on the dimensionality of the support of minimizers [6]. Carrillo presented conditions (sharp in some cases) on the potential that guarantee existence of global minimizers. He also connected the optimality conditions with nonlocal obstacle problems [10, 12] .

DEGOND presented intriguing ideas on reconciling approaches to collective behavior of rational agents (game theory) and agents subject to dynamical effects as can be modeled by kinetic theory [18, 17]. A striking feature of the model is that kinetic stationary and Nash equilibria coincide. This builds a bridge between the so-called econophysics and more classical approaches of economic theory. In terms of modeling at least it seems that there is a considerable potential for future developments, in a spirit similar to the approach of mean-field games.

1.3.4 Hydrodynamics

LAURENÇOT presented a thorough analysis of the thin-film approximation of the Muskat problem for two immiscible fluids placed on top of each other [24]. In leading order, one obtains a system of two diffusion equations of porous medium type, each of the equations governing one of the layers. Again, the mathematical difficulty is to deal with a coupled system of equations. The structural property that facilitates the analysis is that the system can be written as a gradient flow for one energy functional in a metric that combines both components, and there is one additional Lyapunov functional whose dissipation provides useful estimates. The general situation is thus almost identical to the one discussed in Blanchet's talk, and existence follows by similar methods.

The most impressive result of the talk was the richness found in the asymptotic behavior of solutions. Similarly as for the *scalar* porous medium equation, solutions become self-similar in the long-time limit. However, there exists a whole family of qualitatively different self-similar profiles, with different non-trivial topologies. For instance, the lower fluid might lose connectedness of its support, having the upper fluid penetrate down to the bottom. Obtaining estimates on the rate of convergence is currently an open problem.

In her talk, CHUGUNOVA picks up a classical story from lubrication theory. The thin film approximation for a droplet hanging from a stationary cylinder is considered, which leads to the well-known fourth order thin film equation, plus an additional gravity term. For the lubrication of a flat surface, the entropy and energy estimates derived by Bernis and Friedman [7] give a quite precise estimate on the rate of relaxation to a flat horizontal film. The results presented in this talk went into the opposite direction: general solutions approach the shape of a hanging droplet (in H^1) not faster than on algebraic time scale. This seemingly counter-intuitive result was proven by a clever "inversion" of the classical estimates.

YAO talked about the α-patch problem which is a modification of the surface quasi-geostrophic equation. She presented results on finite-time singularity formation.

1.4 Discretizations and numerical methods

One of the intended focal points of the meeting was to discuss the role of the entropy method for finite-dimensional systems, in particular for difference equations arising in discretizations of PDEs with a known entropy structure. The main motivation for this is the design of *structure preserving numerical schemes* that inherit a discretized version of the entropy structure of the original evolution equation. Tthe number of speakers addressing this topic turned out to be smaller than expected. Still, several conceptually very interesting approaches have been presented.

WOLFRAM presented a fully Lagrangian discretization of non-local aggregation and drift equations. Thanks to its Lagrangian nature, the scheme automatically preserves the solution's non-negativity and total mass, and the deformation of the initial mesh provides a nice intuitive picture of the transport underlying the evolution of the density. Moreover, the scheme is "automatically adaptive" in the sense that the mesh is finer in regions where the mass density is high. Thus, the neighborhood of blow-up points are well resolved by the scheme. In practice, the key difficulty is the initialization of the scheme, which requires the solution of a Monge-Ampere equation. The originally rather easy idea turned into a long-term project with manifold unexpected technical difficulties. There are many possibilities for further extensions and for rigorous numerical analysis.

CRAIG talked about a numerical scheme for nonlocal-interaction equations which is inspired by the established *blob method* from computational fluid dynamics [16]. The method is based on the approximate calculation of particle trajectories, where the force exerted on a given particle is not simply the superposition of the forces generated by all of the other particles as point sources, but rather an averaged quantity. Roughly speaking, the point sources are replaced by spatially extended (but still narrowly supported) "blobs". Thanks to this weak averaging, the is method convergent of arbitrary order, provided the initial datum is sufficiently regular.

Finite-volume discretizations for several classes of non-linear drift-diffusion equations were discussed by FILBET. Choosing the discrete fluxes in a suitable way, it can be shown that the approximations produced by the fully discrete scheme inherit the entropy dissipation properties of the original solutions, at least qualitatively. Indeed, the respective entropy decays exponentially fast to its minimum in numerical experiments, and this is justified analytically by proving discrete versions of the entropy-entropy dissipation estimates. Currently, the results remain qualitative in the sense that the provable rate of dissipation for the entropy in the discrete setting is typically different from the known optimal rate of decay of the original equation. This is due to the non-trivial geometry of the mesh, which makes it extremely hard to obtain sharp constants in the discrete functional inequalities.

Finally, it should be mentioned that structure preserving discretization of gradient flows also played a major role in the talk of MAAS, [26, 22], which has been reviewed above in the context of applications to reaction-diffusion equations. A consistent framework has been developed to give sense to, e.g., transportation distances between probability measures on graphs, the curvature of discrete manifolds, and the modulus of convexity for functionals on discrete spaces. The approach is very intuitive, and the calculus that has been developed in this framework has various interesting applications. For instance, it allows to prove functional inequalities for functions on graphs, like discretized versions of the log-Sobolev or Talagrand inequalities. The resulting discrete inequalities are very similar to the ones presented by Filbet, but the relation between the seemingly disjoint approaches still needs to be clarified.

2 Progress Made and Outcome of the Meeting

There has been a remarkable progress in the field over the past four years, since the previous BIRS workshop on a similar topic. Mathematical developments led to a large number of publications, many of them authored by young researchers. There has also been a significant broadening of the field and a shift of focus. While previously the focus has been on single equations, gradient flows in Wasserstein spaces and on specific applications, like the Keller-Segel system, now there is a variety of systems being studied by a broader range of techniques, as clear already from the talks described above. The entropy methods have found their way to discrete descriptions of the systems and remarkable structures have been discovered. The spectrum of applications and relevant models that have some shared mathematical structure has also increased.

The workshop was a great opportunity for researchers to learn about these developments and share their insights and perspective. One of the challenges is be keep a scientific community of people with such a large array of interests united, particularly as far as applications are concerned. We feel that the workshop has accomplished a lot towards that goal.

The workshop has also been an opportunity for many participants to continue existing collaboration on various projects and to initiate some new ones. The organizers did not hear that some spectacular conjecture had been solved during the meeting, but this is also something not so common in the area. However, we have good hope that the meeting will provide a serious boost to the various research directions including ones that have not been mentioned above.

The variety of open problems and emerging mathematical questions should be a clear signal for attracting new PhD students and young researchers in the area of entropy methods and related methods. In the next years, a special effort in that direction is expected from senior participants, in order to promote the topic.

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