



SPIGL'20



Joint Structures and Common Foundation of Statistical Physics, Information Geometry and Inference for Learning

26<sup>th</sup> July to 31<sup>st</sup> July 2020

<https://franknielsen.github.io/SPIG-LesHouches2020/>



## Title

# Joint Structures and Common Foundation of Statistical Physics, Information Geometry and Inference for Learning

## Subject


The conference will deal with the following topics:


- **Geometric Structures of Statistical Physics and Information**
  - Statistical Mechanics and Geometric Mechanics
  - Thermodynamics, Symplectic and Contact Geometries
  - Lie groups Thermodynamics
  - Relativistic and continuous media Thermodynamics
  - Symplectic Integrators
- **Physical structures of inference and learning**
  - Stochastic gradient of Langevin's dynamics
  - Information geometry, Fisher metric and natural gradient
  - Monte-Carlo Hamiltonian methods
  - Variational inference and Hamiltonian controls
  - Boltzmann machine


## Dates

26th July to 31st July 2020

Ecole de Physique des Houches

 <https://houches.univ-grenoble-alpes.fr/>

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## Organizers

**Frédéric Barbaresco**, THALES, KTD PCC, Palaiseau

**Silvère Bonnabel**, Mines ParisTech, CAOR, Paris

**Géry de Saxcé**, Université de Lille, LaMcube, Lille

**François Gay-Balmaz**, Ecole Normale Supérieure Ulm, CNRS & LMD, Paris

**Bernhard Maschke**, Université Claude Bernard, LAGEPP, Lyon

**Eric Moulines**, Ecole Polytechnique, CMAP, Palaiseau

**Frank Nielsen**, Ecole Polytechnique, LIX, Palaiseau & SONY CSL, Tokyo

## Scientific Rational

In the middle of the last century, Léon Brillouin in "The Science and The Theory of Information" or André Blanc-Lapierre in "Statistical Mechanics" forged the first links between the Theory of Information and Statistical Physics as precursors.

In the context of Artificial Intelligence, machine learning algorithms use more and more methodological tools coming from the Physics or the Statistical Mechanics. The laws and principles that underpin this Physics can shed new light on the conceptual basis of Artificial Intelligence. Thus, the principles of Maximum Entropy, Minimum of Free Energy, Gibbs-Duhem's Thermodynamic Potentials and the generalization of François Massieu's notions of characteristic functions enrich the variational formalism of machine learning. Conversely, the pitfalls encountered by Artificial Intelligence to extend its application domains, question the foundations of Statistical Physics, such as the construction of stochastic gradient in large dimension, the generalization of the notions of Gibbs densities in spaces of more elaborate representation like data on homogeneous differential or symplectic manifolds, Lie groups, graphs, tensors, ....

Sophisticated statistical models were introduced very early to deal with unsupervised learning tasks related to Ising-Potts models (the Ising-Potts model defines the interaction of spins arranged on a graph) of Statistical Physics. and more generally the Markov fields. The Ising models are associated with the theory of Mean Fields (study of systems with complex interactions through simplified models in which the action of the complete network on an actor is summarized by a single mean interaction in the sense of the mean field).

The porosity between the two disciplines has been established since the birth of Artificial Intelligence with the use of Boltzmann machines and the problem of robust methods for calculating partition function. More recently, gradient algorithms for neural network learning use large-scale robust extensions of the natural gradient of Fisher-based Information Geometry (to ensure reparameterization invariance), and stochastic gradient based on the Langevin equation (to ensure regularization), or their coupling called "Natural Langevin Dynamics".

Concomitantly, during the last fifty years, Statistical Physics has been the object of new geometrical formalizations (contact or symplectic geometry, ...) to try to give a new covariant formalization to the thermodynamics of dynamic systems. We can

mention the extension of the symplectic models of Geometric Mechanics to Statistical Mechanics, or other developments such as Random Mechanics, Geometric Mechanics in its Stochastic version, Lie Groups Thermodynamic, and geometric modeling of phase transition phenomena.

Finally, we refer to Computational Statistical Physics, which uses efficient numerical methods for large-scale sampling and multimodal probability measurements (sampling of Boltzmann-Gibbs measurements and calculations of free energy, metastable dynamics and rare events, ...) and the study of geometric integrators (Hamiltonian dynamics, symplectic integrators, ...) with good properties of covariances and stability (use of symmetries, preservation of invariants, ...). Machine learning inference processes are just beginning to adapt these new integration schemes and their remarkable stability properties to increasingly abstract data representation spaces.

Artificial Intelligence currently uses only a very limited portion of the conceptual and methodological tools of Statistical Physics. The purpose of this conference is to encourage constructive dialogue around a common foundation, to allow the establishment of new principles and laws governing the two disciplines in a unified approach. However, it is also about exploring new « chemins de traverse ».

	27-jul	28-jul	29-jul	30-jul	31-jul
09.00-09.30	Langevin Dynamics : Gyrfi de Szecs Eric Moulines	Geometric Mechanics: Galilean Mechanics & Thermodynamics Gyrfi de Szecs	Thermodyn. efficiency implies predictive inference Suzanne Sidi	Non-Equilibrium Thermodynamic Geometry: A variational approach to open systems François Gay-Balmaz	On statistical distances and information geometry for proper scoring Frank Nielsen
09.30-10.00	Coffee Break	Coffee Break	Exponential Family by Representation Theory Karel Tsig	Coffee Break	Coffee Break
10.00-10.30					
10.30-11.00	Langevin Dynamics : Gyrfi de Szecs Eric Moulines	Geometric Mechanics: Squire-Cuntz Lie Groups Thermodynamic Machine Learning Frederic Barbresco	Poisons Session	Non-Equilibrium Thermodynamic Geometry: A Homospagous Thermodynamic Approach Allyn van der Schaaf	Computational Information Geometry Information Geometry in Convex Spaces Giovanni Piccini
11.00-11.30					
11.30-12.00					
12.00-12.30	Lunch Break	Lunch Break	Lunch Break	Lunch Break	Lunch Break
12.30-13.00					
13.00-13.30	Learning Physics from Data Francisco Chinesta	Coverant Momentum Map Thermodynamics Girfeco Chirco		Dirac structures in Thermodynamics Hiroaki Yoshizawa	
13.30-14.00					
14.00-14.30	Info. Geometry and Integrable Hamiltonian Jean-Pierre Francoise	Mechanics of the probability simplex Luigi Malagò		Port Thermodynamic Systems Control Bernhard Meschede	
14.30-15.00					
15.00-15.30	Coffee Break	Coffee Break		Coffee Break	
15.30-16.00	Schrodinger's problem, HJB equations Jean-Claude Zenerlin	Diffecological Fisher Metric Hiroki Ueda	Free Time	Computational dynamics of r multibody-fluid system Zdravko Torzo	
16.00-16.30					
16.30-17.00	The Bracket Geometry of Flows and Diffusions Alessandro Berti	Contact geometry and thermodynamical systems Mauricio de Leon		Information Geometry and Quantum Fields Kevin Grosvenor	
17.00-17.30	Sampling and statistical physics via symmetry Steve Hutzman	Deep Learning as Optimal Control Elena Cuffaro		Learning with Few Labeled Data Patrick Chaudhuri	
17.30-18.00					
18.00-18.30					
18.30-19.00	Cocktail				
19.00-19.30					
19.30-20.00	Dinner	Dinner	Dinner	Dinner	
20.00-20.30					
20.30-21.00		SSD Jean-Marc Sourlas's Book 50th Birthday Gyrfi de Szecs & Charles-Michel Maré		GS21 Paris 2021 Announcement Frederic Barbresco & Frank Nielsen	
21.00-21.30					

## LIST OF ABSTRACTS

MONDAY JULY 27<sup>th</sup> 2020

### Langevin Dynamics : Old and News

**Eric Moulines**

#### Abstract:

*In this keynote, we study a method to sample from a target distribution having a positive density with respect to the Lebesgue measure, known up to a normalization factor. This method is based on the Euler discretization of the overdamped Langevin stochastic differential equation associated with the target distribution. For both constant and decreasing step sizes in the Euler discretization, we obtain non-asymptotic bounds for the convergence to the target distribution in Wasserstein and total variation distance. A particular attention is paid to the dependency on the dimension  $d$ , to demonstrate the applicability of this method in the high dimensional setting.*

#### References:

- [1] A. Durmus, E. Moulines, Non asymptotic convergence analysis for the unadjusted Langevin algorithm, the Annals of Applied Probability, 2017
- [2] Cheng, X., Chatterji, N. S., Bartlett, P. L., & Jordan, M. I. (2018), Underdamped Langevin MCMC: A non-asymptotic analysis, In Conference on Learning Theory (pp. 300-323).
- [3] Cheng, X., Chatterji, N. S., Abbasi-Yadkori, Y., Bartlett, P. L., & Jordan, M. I. (2018). Sharp convergence rates for Langevin dynamics in the nonconvex setting. arXiv preprint arXiv:1805.01648.
- [4] Mou, W., Ma, Y. A., Wainwright, M. J., Bartlett, P. L., & Jordan, M. I. (2019). High-order Langevin diffusion yields an accelerated MCMC algorithm. arXiv preprint arXiv:1908.10859.
- [5] Durmus, A., & Moulines, E. (2019). High-dimensional Bayesian inference via the unadjusted Langevin algorithm. Bernoulli, 25(4A), 2854-2882.

### Learning Physics from Data


**Francisco Chinesta**


#### Abstract:


*Acquiring knowledge from data can be performed in a supervised or an unsupervised way. Particular and still open difficulties concern the data themselves: useful, useless, ...; their completeness with respect to the phenomena that we are trying to model (explain), the discovering of the particular form that variables combine to act on the targeted output. Modelling in form of more or less complex regressions can be performed from panoply of techniques, however, in physics first principles must be preserved, fact the enforce constraints but at the same time reduces the amount of need data to perform the learning. Finally, learning will be thermodynamically approached.*

#### References:

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- [1] F. Chinesta, E. Cueto, E. Abisset-Chavanne, J.L. Duval, F. El Khaldi, *Virtual, Digital and Hybrid Twins: A New Paradigm in Data-Based Engineering and Engineered Data*, *Archives of Computational Methods in Engineering*, 27, 105-134, 2020.
- [2] A. Reille, N. Hascoet, C. Ghnatios, A. Ammar, E. Cueto, J.L. Duval, F. Chinesta, R. Keunings, *Incremental dynamic mode decomposition: A reduced-model learner operating at the low-data limit*, *C. R. Mécanique*, 347, 780-792, 2019.
- [3] J.A. Lee, M. Verleysen. *Nonlinear dimensionality reduction*. Springer, New York, 2007.
- [4] D. Gonzalez, F. Chinesta, E. Cueto. *Thermodynamically consistent data-driven computational mechanics*. *Continuum Mech. Thermodynamics*, <https://doi.org/10.1007/s00161-018-0677-z>, 2018.
- [5] D. Gonzalez, F. Chinesta, E. Cueto. *Learning corrections for hyperelastic models from data*. *Frontiers in Materials - section Computational Materials Science*, In press.

### Information Geometry and Integrable Systems

Jean-Pierre Francoise

#### Abstract:

We analyze in parallel the (open) Toda-Lattice and the finite Peakons\anti-Peakons system. Their scattering theory relies on a theorem of Stieljes as shown by J. Moser (1975) and R. Beals; D. Sattinger; J. Szmigielski (1999, 01,05,07). We show that both these systems linearize in the setting of Information Geometry. This can be seen as revisiting of previous works of Nakamura, Nakamura and Kodama (1994-1995) where the tau-function of the Toda-Lattice was discovered using Information Geometry.

#### References:

- [1] Beals, Richard; Sattinger, David H.; Szmigielski, Jacek, *Multipeakons and the classical moment problem*. *Adv. Math.* 154 (2000), no. 2, 229–257.
- [2] Beals, Richard; Sattinger, David H.; Szmigielski, Jacek, *Peakons, strings, and the finite Toda lattice*. *Comm. Pure Appl. Math.* 54 (2001), no. 1, 91–106.
- [3] S.I. Amari, *Information Geometry and its Applications*, *Applied Mathematical Sciences*, vol. 194, Springer Japan (2016).
- [4] Nakamura, Yoshimasa, *A tau-function for the finite Toda molecule, and information spaces*. *Symplectic geometry and quantization* (Sanda and Yokohama, 1993), 205–211, *Contemp. Math.*, 179, Amer. Math. Soc., Providence, RI, 1994.
- [5] Nakamura, Yoshimasa; Kodama, Yuji, *Moment problem of Hamburger, hierarchies of integrable systems, and the positivity of tau-functions*. *KdV '95* (Amsterdam, 1995). *Acta Appl. Math.* 39 (1995), no. 1-3, 435–443.
- [6] *A Series of Modern Surveys in Mathematics*, 64. Springer, Cham, 2017.

### Schroedinger's problem, HJB equations

Jean-Claude Zambrini

#### Abstract:

In 1931-2 Schrödinger formulated an unorthodox problem of classical statistical physics, motivated by his worries about the interpretation of quantum theory. The framework founded on

the solution of his problem is a curious anticipation of Feynman's path integral approach (but probabilistically sound) where Hamilton-Jacobi-Bellman equations are central. We shall describe the connections between these ideas. And why Schrödinger's problem is regarded today as a regularized Monge – Kantorovich problem, at the foundation of Mass transportation theory.

References:

- [1] E. Schrödinger, Sur la théorie relativiste de l'électron et l'interprétation de la mécanique quantique, Ann. Inst. H. Poincaré 2 (1932), 269
- [2] J. C Zambrini, Variational processes and stochastic versions of mechanics, J. Math. Physics, 27(9), Sept 1986, p 2307
- [3] J.C. Zambrini, On the geometry of the Hamilton-Jacobi-Bellman equation, Journal of Geometric Mechanics 1(3), Sept 2009, p369
- [4] C. Leonard, A survey of Schrödinger's problem and some of its connections with optimal transport, Discrete and continuous dynamical systems A-34(4), 2014, p1533-74. Special issue on Optimal transport and applications.
- [5] J.C. Zambrini, The research program of Stochastic Deformation (with a view toward Geometric Mechanics), in Stochastic Analysis : A Series of Lectures, Editors R.C. Dalang, M. Dozzi, F. Flandoli, F. Russo. Progress in Probability Vol 68, 359-393, Springer Basel 2015.

### The Bracket Geometry of Measure-Preserving Flows and Diffusions

**Alessandro Barp**

Abstract:

Following ideas from Koszul, de Rham, and Weinstein, we discuss the canonical geometry generated by a target measure [1-2], and derive characterisations of measure-preserving flows that allows us to extend the complete recipe of stochastic gradient MCMC to manifolds [3].

References:

- [1] Weinstein, Alan. The modular automorphism group of a Poisson manifold. Journal of Geometry and Physics 23.3-4 (1997): 379-394.
- [2] Koszul, Jean-Louis. Crochet de Schouten-Nijenhuis et cohomologie. Astérisque 137 (1985): 257-271.
- [3] Ma, Yi-An, Tianqi Chen, and Emily Fox. A complete recipe for stochastic gradient MCMC. Advances in Neural Information Processing Systems. 2015.

### Sampling and statistical physics via symmetry

**Steve Huntsman**

Abstract:

In the first part of the talk, we describe how elementary considerations of symmetry (viz., the Lie group preserving a probability measure) lead to a unifying picture of Markov chain Monte Carlo algorithms, including an apparently new parallel MCMC algorithm that converges faster than state-of-the-art techniques. In the second part of the talk, we use basic physical symmetries to parsimoniously derive an effective temperature for steady-state systems with finitely many states. We then show how this construction can be adapted to archetypal physical systems (viz.,

Anosov flows) and produce results suggesting how it may ultimately be used to recover physics from data as well as for more conceptually straightforward descriptive tasks.

References:

[1] Huntsman, S. Fast Markov chain Monte Carlo algorithms via Lie groups. AISTATS (2020).

<https://arxiv.org/abs/1901.08606>

[2] Huntsman, S. Effective statistical physics of Anosov systems.

<https://arxiv.org/abs/1009.2127>



TUESDAY JULY 28<sup>th</sup> 2020

**Geometric Mechanics:  
Galilean Mechanics & Thermodynamics of Continua**

**Géry de Saxcé**

Abstract:

Inspired from the relativistic approaches by Souriau [1] and Vallée [2], we propose a geometrization of the thermodynamics of dissipative continua compatible with the Galilean physics [3]. With this aim in view, we emphasize the role of Bargmann's group [4], a central extension of Galileo's one [5]. Originally introduced for applications to quantum mechanics, it turns out to be also very useful in thermodynamics.

References:

- [1] Souriau, J.-M., 1978. Thermodynamique relativiste des fluides. Rendiconti del Seminario Matematico Università e Politecnico di Torino. 35, 21–34.
- [2] Vallée, C., 1981. Relativistic thermodynamics of continua, International Journal of Engineering Science, 19, 589–601.
- [3] de Saxcé, G., Vallée, C., 2012. Bargmann Group, Momentum Tensor and Galilean invariance of Clausius-Duhem Inequality. International Journal of Engineering Science. 50, 216–232.
- [4] Bargmann, V., 1954. On unitary representation of continuous groups. Annals of Mathematics, 59(1), 1–46.
- [5] de Saxcé, G., Vallée, C., 2010. Construction of a central extension of a Lie group from its class of symplectic cohomology. Journal of Geometry and Physics. 60, 165–174.

**Geometric Mechanics:  
Souriau-Casimir Lie Groups Thermodynamics & Machine Learning**

**Frédéric Barbaresco**

Abstract:

50 years ago, Jean-Marie Souriau invented a “Lie Groups Thermodynamics” model in Statistical Mechanics in his book on Geometric Mechanics, entitled “Structure des systèmes dynamiques” ([http://www.jmsouriau.com/structure\\_des\\_systemes\\_dynamiques.htm](http://www.jmsouriau.com/structure_des_systemes_dynamiques.htm)) and in [1]. We will extend this model in the framework of Information Geometry for Lie Group Statistics and Lie Group Machine Learning. Based on this Symplectic model of Statistical Physics, we can define a Souriau-Koszul-Fisher Metric elaborated on covariant Souriau Gibbs density. Finally, we will propose a new geometric definition of Entropy as a generalized Casimir invariant function in coadjoint representation where Souriau cocycle is a measure of the lack of equivariance of the moment mapping. Lie algebra cohomology, coadjoint orbit methods, and affine representation of Lie Group and Lie Algebra are the main structures used for this elaboration.

References:

- [1] Jean-Marie Souriau, Mécanique statistique, groupes de Lie et cosmologie, Colloques int. du CNRS numéro 237. Aix-en-Provence, France, 24–28, pp. 59–113, 1974 (English translation: [https://www.academia.edu/42630654/Statistical\\_Mechanics\\_Lie\\_Group\\_and\\_Cosmology\\_1st\\_part\\_Symplectic\\_Model\\_of\\_Statistical\\_Mechanics](https://www.academia.edu/42630654/Statistical_Mechanics_Lie_Group_and_Cosmology_1st_part_Symplectic_Model_of_Statistical_Mechanics) )

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[2] Frédéric Barbaresco; François Gay-Balmaz, F. Lie Group Cohomology and (Multi)Symplectic Integrators: New Geometric Tools for Lie Group Machine Learning Based on Souriau Geometric Statistical Mechanics. *Entropy* 2020, 22, 498.

<https://www.mdpi.com/1099-4300/22/5/498>

[3] Frédéric Barbaresco; Lie Group Statistics and Lie Group Machine Learning Based on Souriau Lie Groups Thermodynamics & Koszul-Souriau-Fisher Metric: New Entropy Definition as Generalized Casimir Invariant Function in Coadjoint Representation. *Entropy* 2020, 22, 642.

<https://www.mdpi.com/1099-4300/22/6/642>

[4] Charles-Michel Marle. From Tools in Symplectic and Poisson Geometry to J.-M. Souriau's Theories of Statistical Mechanics and Thermodynamics. *MDPI Entropy*, 18, 370, 2016

<https://www.mdpi.com/1099-4300/18/10/370>

[5] Jean-Louis Koszul, *Introduction to Symplectic Geometry*, SPRINGER, 2019

<https://link.springer.com/book/10.1007%2F978-981-13-3987-5>

### Covariant Momentum Map Thermodynamics for Parametrized Field Theories

Goffredo Chirco

#### Abstract:

Inspired by Souriau's symplectic generalization of Gibbs equilibrium in Lie group thermodynamics, we define a general-covariant notion of Gibbs state for parametrised field theories, in terms of the covariant momentum map associated with the lifted action of the diffeomorphisms group on the extended multi-symplectic phase space. The equilibrium entangles gauge and dynamic information carried by the theory. We investigate how physical equilibrium, hence time evolution, emerges from such a state and the role of the gauge symmetry in the thermodynamic description.

#### References:

[1] J.-M. Souriau, *Structure des Systèmes Dynamiques*, ; Dunod: Malakoff, France (1969).

[2] M. J. Gotay, J. Isenberg, J. E. Marsden, and R. Montgomery, *Momentum Maps and Classical Relativistic Fields. Part I-II-III*, arXiv:physics/9801019 [math-ph].

[3] C. J. Isham and K. V. Kuchař, *Representations of Spacetime Diffeomorphisms. I. Canonical Parametrized Field Theories*, *Ann. Phys.* 164, 288-315, (1985).

[4] G. Chirco, T. Josset, C. Rovelli, *Statistical mechanics of reparametrization-invariant systems. It takes three to tango*. *Class. Quantum Gravity* 2016, 33, 045005.

[5] A. Connes, C. Rovelli, *Von Neumann Algebra Automorphisms and Time-Thermodynamics Relation in General Covariant Quantum Theories*, *Class. Quant. Grav.* 11, 2899 - 2918 (1994).

### Mechanics of the probability simplex

Luigi Malagò

#### Abstract:

The framework of classical Mechanics is a finite-dimensional Riemannian manifold. Information Geometry describes statistical models as manifolds of probability distributions, endowed with a Riemannian metric given by the Fisher matrix and with a dually flat connection. In this talk we study the mechanics of the probability simplex using an approach based on non parametric

*Information Geometry. We start by defining the statistical bundle as the set of couples of a positive probability density and a random variable centered in the density, and we express densities in the affine atlases of exponential charts. We compute velocities and accelerations of a one-dimensional statistical model using the canonical dual pair of parallel transports and define Lagrangian and Hamiltonian mechanics on the bundle. Following our mechanical approach, we are able to define a coherent theory of second-order differential equations which can be used to define different accelerated natural gradient dynamics on the probability simplex.*

References:

- [1] Shun-ichi Amari and Hiroshi Nagaoka. *Methods of information geometry*, American Mathematical Society. Translated from the 1993 Japanese original by Daishi Harada.
- [2] Lev D. Landau and Eugenij M. Lifshits. *Course of theoretical physics. mechanics.*, 3rd ed., vol. I, Butterworth-Heinemann, 1976
- [3] Giovanni Pistone and Carlo Sempì. An infinite-dimensional geometric structure on the space of all the probability measures equivalent to a given one. *Ann. Statist.* 23 (1995), no. 5, 1543–1561
- [4] Giovanni Pistone. Lagrangian function on the finite state space statistical bundle, *Entropy* 20 (2018), no. 2, 139
- [5] Andre Wibisono, Ashia C. Wilson, and Michael I. Jordan. A variational perspective on accelerated methods in optimization, *Proceedings of the National Academy of Sciences* 113 (2016), no. 47

### Diffeological Fisher Metric

Hông Vân Lê

Abstract:

*Diffeological Fisher metric is a natural generalization of the Fisher metric on parametrized statistical models to the case of diffeological statistical models, which are statistical models endowed with a compatible diffeology. In my lecture, I shall discuss properties of the diffeological Fisher metric, in particular a diffeological version of the Cramér-Rao inequality.*

References:

- [1] Amari S., and Nagaoka H., *Methods of Information Geometry*, Translations of Mathematical Monographs 191, Amer. Math. Soc.: Providence, RI, USA, 2000.
- [2] Ay N., Jost J., Lê H.V., Schwachhöfer L., *Information geometry*, Springer Nature: Cham, Switzerland, 2017.
- [3] Iglesias-Zemmour P., *Diffeology*, Amer. Math. Soc.: Providence, RI, USA, 2013.
- [4] Jost J., Lê H.V., Luu D.H. and Tran T.D., *Probabilistic mappings and Bayesian nonparametrics*, 2019, arXiv:1905.11448.
- [5] Lê H.V., *Diffeological Statistical Models, the Fisher Metric and Probabilistic Mappings*, *Mathematics* 2020, 8, 167; doi:10.3390/math8020167.

### Contact geometry and thermodynamical systems

Manuel de León

Abstract:

Using contact geometry we give a new characterization of a simple but important class of thermodynamical systems which naturally satisfy the first law of thermodynamics (total energy preservation) and the second law (increase of entropy). We clarify its qualitative dynamics, the underlying geometrical structures and we show how to use discrete gradient methods.

References:

- [1] A Bravetti: Contact geometry and thermodynamics. *Int. J. Geom. Methods Mod. Phys.*, 16 (supp01):1940003, October 2018.
- [2] F Gay-Balmaz, H Yoshimura: A Lagrangian variational formulation for nonequilibrium thermodynamics. Part I: Discrete systems. *Journal of Geometry and Physics*, 111:169–193, January 2017.
- [3] M de León, M Lainz Valcázar: Contact Hamiltonian systems. *Journal of Mathematical Physics* (2019) 60 (10), 102902
- [4] AA Simoes, DM de Diego, M de León, ML Valcázar: On the geometry of discrete contact mechanics. *arXiv preprint arXiv:2003.11892*
- [5] AA Simoes, M de León, ML Valcázar, DM de Diego: Contact geometry for simple thermodynamical systems with friction. *arXiv preprint arXiv:2004.01989*

## Deep learning as optimal control and structure preserving deep learning

**Elena Celledoni**

Abstract:

Over the past few years, deep learning has risen to the foreground as a topic of massive interest, mainly as a result of successes obtained in solving large-scale image processing tasks. There are multiple challenging mathematical problems involved in applying deep learning.

We consider recent work of Haber and Ruthotto 2017 and Chang et al. 2018, where deep learning neural networks have been interpreted as discretisations of an optimal control problem subject to an ordinary differential equation constraint. We review the first order conditions for optimality, and the conditions ensuring optimality after discretisation. There is a growing effort to mathematically understand the structure in existing deep learning methods and to systematically design new deep learning methods to preserve certain types of structure in deep learning. Examples are invertibility, orthogonality constraints, or group equivariance, and new algorithmic frameworks based on conformal Hamiltonian systems and Riemannian manifolds.

References:

- [1] Martin Benning, Elena Celledoni, Matthias J. Ehrhardt, Brynjulf Owren, Carola-Bibiane Schönlieb, Deep learning as optimal control problems: models and numerical methods, <https://arxiv.org/abs/1904.05657>
- [2] Elena Celledoni, Matthias J. Ehrhardt, Christian Etmann, Robert I McLachlan, Brynjulf Owren, Carola-Bibiane Schönlieb, Ferdia Sherry, Structure preserving deep learning, <https://arxiv.org/abs/2006.03364>

## SSD Jean-Marie Souriau's Book 50th Birthday

**Gery de Saxcé & Charles-Michel Marle**

Abstract:

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« *Structure des systèmes dynamiques* » [1], now translated into English [2], is a work with an exceptional wealth which, fifty years after its publication, is still topical. We shall intend to highlight author's most creative and promising ideas on the symplectic geometry and its applications: both classical and relativistic mechanics, geometric quantization and Lie group thermodynamics.

References:

[1] Souriau, J.-M., *Structure des systèmes dynamique*. Dunod, collection Dunod Université, Paris 1970. Réimprimé par les éditions Jacques Gabay, Paris.

[2] Souriau, J.-M., *Structure of Dynamical Systems. A Symplectic View of Physics*. Translated by C. H. Cushman-de Vries. Translation Editors R. H. Cushman and G. M. Tuynman. *Progress in Mathematics* Volume 149, Birkhäuser, Boston, 1997.



## WEDNESDAY JULY 29<sup>th</sup> 2020

### Thermodynamic efficiency implies predictive inference

**Susanne Still**

Abstract:

Machine learning is a core ingredient of contemporary statistical data analysis. As with statistics, the foundations are mathematical in nature, often based on “ad hoc” measures. But learning is a natural phenomenon occurring in the physical world. Therefore, we would like to have a physics based explanation. We need to understand how observers choose their strategy for how to represent, and adapt to, the data they receive. Indulge, for a moment, the following hypothesis: observers choose their strategy such that the best physical implementation of abstract rules specifying the strategy could come as close as possible to the physical limits imposed on information processing. This postulate would open a door to “derive” learning methods from “physics”, simply by minimizing a physical bound over all possible rules, thereby finding the strategy optimal with respect to the limitation expressed by the bound. Here, I show that this can be done for thermodynamic limits: energy efficiency implies predictive inference, a strategy that lies at the heart of machine learning.

References:

- [1] S. Still. Thermodynamic cost and benefit of memory. *Physical Review Letters*, 124(5):050601, 2020
- [2] S. Still, D. A. Sivak, A. J. Bell, and G. E. Crooks. Thermodynamics of prediction. *Physical Review Letters*, 109(12):120604, 2012
- [3] S. Still, Information theoretic approach to interactive learning, *EPL* 85, 28005, 2009
- [4] S. Still, Information Bottleneck Approach to Predictive Inference, *Entropy* 16(2):968-989, 2014
- [5] S. Still, Lossy is lazy, *Workshop on Information Theoretic Methods in Science and Engineering* (pp. 17-21), University of Helsinki, 2014.

### Exponential Family by Representation Theory

**Koichi Tojo**

Abstract:

Exponential families play an important role in the field of information geometry. By definition, there are infinitely many exponential families. However, only a small part of them are widely used. We want to give a framework to deal with these “good” families. In light of the observation that the sample space of most of them are homogeneous spaces of certain Lie groups, we proposed a method to construct exponential families on homogeneous spaces by taking advantage of representation theory in [1]. This method generates widely used exponential families such as normal, gamma, Bernoulli, categorical, Wishart, von Mises-Fisher, and hyperboloid distributions. In this talk, we will explain the method, its properties and future works.

References:

- [1] K. Tojo, T. Yoshino, A method to construct exponential families by representation theory, *arXiv:1811.01394v3*.

[2] K. Tojo, T. Yoshino, *On a method to construct exponential families by representation theory*, Geometric Science of Information. GSI2019, Lecture Notes in Computer Science, vol 11712, 147-156 (2019).

## POSTERS SESSION

Poster Authors	Poster Title
Timothée Poudon, Benedict Leinkuhler, Charles Matthews and Tiffany Vaar	Constraint-Based Regularization of Neural Networks
Kevin Grosvenor	Information Geometry and the Effective Field Theory of Flocking
Rita Foresi	A geometric interpretation of stochastic gradient descent in Deep Learning and Restricted Boltzmann Machines
Filipe Dias	Geometric Thermodynamics of Information Processing and Fluctuations
Anis Fradi and Chaïk Samir	Bayesian Inference on Local Distributions of Functions and Multi-dimensional Curves with Spherical HMC Sampling
Carlos Couto, José Mourão, João P. Nunes and Pedro Ribeiro	Connecting Stochastic Optimization with Schrödinger evolution with respect to non-Hermitian Hamiltonians
Emmanuel Chevallier and Nicolas Gugli	Warped statistical models on SE(n): motivation, challenges and generalization on symmetric spaces
Sébastien Boyaval	Viscoelastic flows with conservation laws
Filippo Masi, Ioannis Stefanou, Paolo Vannucci and Victor Maffi-Berthier	Material modeling via Thermodynamics-based Artificial Neural Networks
Nicolas Gugli, Nina Mieland and Alice le Bigant	Geostatistics: a Python package for Geometric Learning and Information Geometry
Haïtem Hajji, Thomas Gerald and Hadi Zaati	Hyperbolic learning of communities on graphs
Goffredo Circo, Luigi Malagò and Giovanni Pistone	Lagrangian and Hamiltonian Dynamics on the Simplex
Hector Javier Hortua, Luigi Malagò and Riccardo Voipi	Calibrating Bayesian Neural Networks with Alpha-divergences and Normalizing Flows
Youssef El Habouz	Semi-supervised Classification of Cells based on GAN
Avetik Karagulyan and Arnak Dalalyan	Bounding the error of discretized Langevin algorithms for non-strongly log-concave targets
Elvis Dohmatob	Universal Lower-Bounds on Classification Error under Adversarial Attacks and Random Corruption
Pierre-Cyril Aubin-Frankowski and Zoltan Szabo	Hard Shape-Constrained Kernel Regression
Bruno Sauvalle	Unsupervised object detection for traffic scene analysis
Paul Ferrand, Alexis Decurtinge, Luis Garcia Ordonez and Maxime Guillaud	Learning the low-dimensional geometry of the wireless channel

THURSDAY JULY 30<sup>th</sup> 2020

**Non-Equilibrium Thermodynamic Geometry:  
A variational perspective on nonequilibrium thermodynamics of closed and open  
systems**

**François Gay-Balmaz**

Abstract:

We survey recent results on the variational formulation of nonequilibrium thermodynamics for finite-dimensional and continuum systems. We illustrate the theory with closed and open systems experiencing friction, heat and mass transfer, and chemical reactions. We show how the theory is used for discretization and as a modeling tool in fluid dynamics.

References:

- [1] F. Gay-Balmaz and H. Yoshimura [2017], A Lagrangian variational formalism for nonequilibrium thermodynamics. Part I: discrete systems, *J. Geom. Phys.*, 111, 169–193.
- [2] F. Gay-Balmaz and H. Yoshimura [2017], A Lagrangian variational formalism for nonequilibrium thermodynamics. Part II: continuum systems, *J. Geom. Phys.*, 111, 194–212.
- [3] F. Gay-Balmaz and H. Yoshimura [2018], Variational discretization of the nonequilibrium thermodynamics of simple systems, *Nonlinearity*, 31(4), 1673.
- [4] F. Gay-Balmaz and H. Yoshimura [2018], A variational formulation of nonequilibrium thermodynamics for discrete open systems with mass and heat transfer, *Entropy*, 20(3), 163.
- [5] F. Gay-Balmaz [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.

**Non-Equilibrium Thermodynamic Geometry:  
A Homogeneous Symplectic Approach**


**Arjan van der Schaft**


Abstract:


Since the early 1970s contact geometry has been recognized as an appropriate geometric framework for thermodynamic systems. In the 2001 paper by Balian and Valentin it was shown how the homogeneous symplectic approach to contact geometry has several advantages, e.g., in switching between energy and entropy representations. In this talk I will show how this approach leads to a geometric formulation of non-equilibrium thermodynamic processes, in terms of Hamiltonian dynamics defined by Hamiltonian functions that are homogeneous of degree one in the co-extensive variables and zero on the homogeneous Lagrangian submanifold describing the state properties. This culminates in the definition of port-thermodynamic systems, and the formulation of interconnection ports with the environment or other systems. This is illustrated on a number of simple examples, indicating its potential for analysis and control.

References:

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- [1] A. van der Schaft, B. Maschke. Geometry of thermodynamic processes. *Entropy*, 20(12):925-947, 2018.
- [2] R. Balian, P. Valentin. Hamiltonian structure of thermodynamics with gauge. *Eur. J. Phys. B*, 21:269–282, 2001.
- [3] A.J. van der Schaft, B. Maschke. About some system-theoretic properties of port-thermodynamic systems. pp. 228--238 in *Geometric Science of Information, Toulouse, France, 2019*, eds. F. Nielsen, F. Barbaresco, *Lecture Notes in Computer Science*, Springer-International, 2019.

### Dirac structures and port-Dirac systems in nonequilibrium thermodynamics

**Hiroaki Yoshimura**

#### Abstract:

A Dirac structure is a unifying notion of symplectic and Poisson structures, which has been widely used in mechanics, in particular, for mechanical systems with nonholonomic constraints. In this talk, we study Dirac structures in nonequilibrium thermodynamics by extending to a class of nonlinear nonholonomic systems. We also clarify the associated variational structures together with some examples of open systems as well as interconnected systems. This is a joint work with Francois Gay-Balmaz.

#### References:

- [1] Gay-Balmaz, F. and H. Yoshimura, A variational formulation of nonequilibrium thermodynamics for discrete open systems with mass and heat transfer, *Entropy*, 20(3), 163; doi: 10.3390/e20030163, 1–26., 2018
- [2] Gay-Balmaz, F. and H. Yoshimura, Variational discretization for the nonequilibrium thermodynamics of simple systems, *Nonlinearity*, in press, 2018
- [3] Gay-Balmaz, F. and H. Yoshimura, Dirac structures in nonequilibrium thermodynamics, *J. Math. Phys.* 59, 012701-29., 2018
- [4] Gay-Balmaz, F. and H. Yoshimura, From Lagrangian mechanics to nonequilibrium thermodynamics: A variational perspective, *Entropy* 21(1), 8; doi: 10.3390/e21010008, 1–39., 2019
- [5] Gay-Balmaz, F. and H. Yoshimura, From variational to bracket formulations in nonequilibrium thermodynamics of simple systems, *arXiv:1904.05958v1*, 11 April 2019

### Port Thermodynamic Systems Control

**Bernhard Maschke**

#### Abstract:

We consider the feedback control of homogeneous Hamiltonian control systems arising in the Hamiltonian modelling of open thermodynamic systems and presented in the talk “Non-Equilibrium Thermodynamic Geometry: A Homogeneous Symplectic Approach”. In this talk we characterize classes of state feedbacks for which the closed-loop system is again Homogeneous Hamiltonian and leaves invariant some closed-loop 1-form and derive some relations with the closed-loop Hamiltonian function.

#### References:



- [1] B. Maschke and A. van der Schaft, Port-thermodynamic systems and the assignment of their structure by feedback, 58th IEEE Conference on Decision and Control will be held Wednesday through Friday, December 11-13, 2019
- [2] A. van der Schaft and B. Maschke, Structure preserving feedback of Port-thermodynamic system 11th IFAC Symposium on Nonlinear Control Systems (NOLCOS 2019), Vienna, Austria, September 4-6, 2019
- [3] A. van der Schaft and B. Maschke, About some system theoretic properties of port-thermodynamic systems, Proc. Geometric Science of Information, Toulouse, France, 27-29 August 2019, F.Nielsen and F. Barbaresco eds., LNCS, volume 11712, Springer
- [4] A.J. van der Schaft and B. Maschke, Geometry of Thermodynamic Processes, Entropy vol. 20, n°12, n° paper 925, Dec. 2018
- [5] H. Ramirez, B. Maschke and Daniel Sbarbaro, Partial stabilization of input-output contact systems on a Legendre submanifold, IEEE Transaction on Automatic Control, Vol. 62, n°3, pp. 1431 - 1437, March 2017

### Computational dynamics of reduced coupled multibody-fluid system in Lie group setting Zdravko Terze

#### Abstract:

We describe a computationally efficient method for simulating dynamics of multibody-fluid system that utilizes symplectic and Lie-Poisson reductions in order to formulate fully coupled dynamical model of the multi-physical system by using solid variables only. Multibody system dynamics is formulated in Lie group setting and integrated with the pertinent integration method, while additional viscous effects are incorporated in the overall model by numerically enforcing Kutta condition.

#### References:

- [1] Arnold, V. I., and Khesin, B. A. Topological Methods in Hydrodynamics. Springer-Verlag, Berlin, Heidelberg, 1998.
- [2] Kanso, E., Marsden, J. E., Rowley, C. W., and Melli-Huber, J. B. Locomotion of articulated bodies in a perfect fluid. Journal of Nonlinear Science 15, 4 (2005), 255–289.
- [3] García-Naranjo, L. C., and Vankerschaver, J. Nonholonomic LL systems on central extensions and the hydrodynamic Chaplygin sleigh with circulation. Journal of Geometry and Physics 73 (2013), 56-69.
- [4] Terze, Z., Müller, A., and Zlatar, D. Lie-group integration method for constrained multibody systems in state space. Multibody System Dynamics 34, 3 (2015), 275–305.
- [5] Shashikanth, B. N., Marsden, J. E., Burdick, J. W., and Kelly, S. D. The Hamiltonian structure of a two-dimensional rigid circular cylinder interacting dynamically with  $N$  point vortices. Physics of Fluids 14, 3 (2002), 1214–1227.

### Information Geometry & Quantum Fields Kevin Grosvenor

#### Abstract:

We study the Fisher metrics associated with a variety of simple systems and derive some general lessons that may have important implications for the application of information geometry in holography. Some sample systems of interest are the classical 2d Ising model and the corresponding 1d free fermion theory, massless scalar instantons, and coherent states of free bosons and fermions.

References:

- [1] Johanna Erdmenger, Kevin T. Grosvenor, and Ro Jefferson. Information geometry in quantum field theory: lessons from simple examples. *SciPost Phys.* 8 (2020) 5, 073. [arXiv:2001.02683]. Inspirehep link: <https://inspirehep.net/literature/1774704>
- [2] Matthias Blau, K.S. Narain, and George Thompson, Instantons, the information metric, and the AdS/CFT correspondence. [arXiv:hep-th/0108122]. Inspirehep link: <https://inspirehep.net/literature/561605>
- [3] Masahiro Nozaki, Shinsei Ryu, and Tadashi Takayanagi. Holographic geometry of entanglement renormalization in quantum field theories. *JHEP* 10 (2012) 193. [arXiv:1208.3469]. Inspirehep link: <https://inspirehep.net/literature/1128036>

## Learning with Few Labeled Data

**Pratik Chaudhari**

Abstract:

The relevant limit for machine learning is not  $N \rightarrow \text{infinity}$  but instead  $N \rightarrow 0$ , the challenge is to build systems that do not require  $N = \text{thousands of labeled data}$ . We will exploit a formal connection of thermodynamics and machine learning to characterize the limits of representation learning in the low-data regime. This theory leads to algorithms that can guarantee good classification performance after the model is transferred onto a new task.

References:

- [1] Chaudhari, Pratik, and Stefano Soatto. "Stochastic gradient descent performs variational inference, converges to limit cycles for deep networks." In *Proc. of the International Conference on Learning and Representations (ICLR)*, 2018. <https://arxiv.org/abs/1710.11029>.
- [2] Gao, Yansong, and Pratik Chaudhari. "A Free-Energy Principle for Representation Learning." In *Proc. of the International Conference of Machine Learning (ICML)*, 2020. <https://arxiv.org/abs/2002.12406>.
- [3] Dhillon, Guneet S., Pratik Chaudhari, Avinash Ravichandran, and Stefano Soatto. "A baseline for few-shot image classification." In *Proc. of the International Conference on Learning and Representations (ICLR)*, 2020. <https://arxiv.org/abs/1909.02729>.

FRIDAY JULY 31<sup>st</sup> 2020

**Computational Information Geometry:  
On statistical distances and information geometry for machine learning**

**Frank Nielsen**

Abstract:

We survey recent progress in the construction of divergences and their induced information geometry with applications to machine learning: First, we provide generalizations of the celebrated Jensen-Shannon divergence [1,2] that is at the heart of Generative Adversarial Networks. Second, we describe some statistical divergences on the Cauchy manifold [3] with their information-geometric structures, and show applications in statistics. Third, we show how to quickly calculate numerically the Siegel distance on the Siegel disk domain using the novel Siegel-Klein model [4] based on Hilbert geometry, and discuss applications in machine learning. Last, we show a simple trick to easily calculate statistical distances between exponential families using legacy software packages [5].

References:

- [1] Frank Nielsen: On a Generalization of the Jensen-Shannon Divergence and the Jensen-Shannon Centroid. *Entropy* 22(2): 221 (2020)
- [2] Frank Nielsen: On the Jensen-Shannon Symmetrization of Distances Relying on Abstract Means. *Entropy* 21(5): 485 (2019)
- [3] Frank Nielsen: On Voronoi diagrams on the information-geometric Cauchy manifolds, *Entropy* (2020)
- [4] Frank Nielsen: Hilbert geometry of the Siegel disk: The Siegel-Klein disk model. *CoRR abs/2004.08160* (2020)
- [5] Frank Nielsen, Richard Nock: Cumulant-free closed-form formulas for some common (dis)similarities between densities of an exponential family. *CoRR abs/2003.02469* (2020)

Coffe Break

**Computational Non-Parametric Information Geometry  
Information Manifold modeled with Orlicz Spaces**

**Giovanni Pistone**

Abstract:


One of the possible non-parametric version of Information Geometry with infinite sample space assumes strictly positive densities whose logarithm belongs to an Orlicz space. In this way, the full structure of the affine Hessian statistical manifold can be rigorously derived. After a brief summary of this old theory, I will discuss some recent developments:


1. The extension of the Orlicz space modeling to the statistical bundle;
2. The use of Orlicz-Sobolev spaces to allow for smoothness of the densities;
3. The special features of the finite-dimensional Gaussian Space.


References:

- [1] J. Musielak (1983) Chapter II of *Orlicz spaces and modular spaces*. Springer

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- [2] P. Malliavin (1995) Chapter V of *Integration and Probability*\_ Springer  
[3] G. Pistone. (2018) *Information Geometry of the Gaussian Space in Information Geometry and Its Applications*\_ Springer  
[4] M.J. Wainwright (2019) Chapter 2 of *High-dimensional Statistics*\_ CUP  
[5] G. Pistone (2020) *Information Geometry of smooth densities on the Gaussian space: Poincaré inequalities*. arXiv:2002.12871

