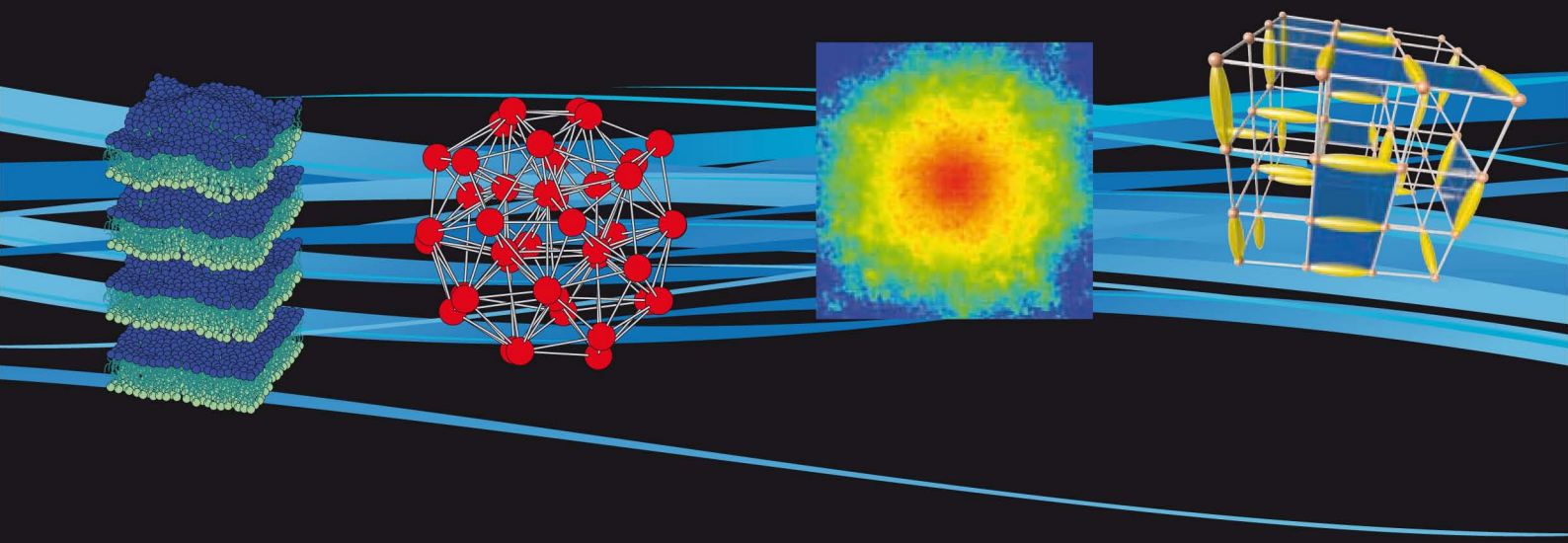
Laboratoire de Physique Théorique



UMR 5152 CNRS & Université Toulouse III

Scientific Report

Bilan Scientifique

2005-2009

Contents

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Équipe Physique Statistique des Systèmes Complexes (PhyStat)

The PhyStat group addresses a large variety of problems using the analytical and numerical tools of statistical physics, and in particular, out of equilibrium statistical physics. Over the last ten years, it has developed a strong activity in the field of soft condensed matter physics (ionic fluids, polymers, lipidic films...) and biophysics of the cell membrane, collaborating and sharing contracts with several experimental groups of biologists and physicists. The PhyStat group also has a strong expertise in the applications of stochastic processes in various contexts (diffusing processes in random media, theory of signals, theory of competition, optimization problems...), and the physics of long-range interacting systems (with applications to turbulence, astrophysics, chemotaxis...).

The PhyStat group is headed by David S. Dean (PR1 & IUF) and the other permanent researchers are Pierre-Henri Chavanis (CR1), Nicolas Destainville (MCF), Manoel Manghi (MCF), John Palmeri (CR1), and Clément Sire (DR2, head of LPT). Non permanent staff includes two post-docs, Sahin Buyukdagli and Luca Delfini, and four PhD students, Thomas Portet (LPT-IPBS collaboration), Lorand Horvath (LPT-University of Cluj-Napoca collaboration), Julien Sopik (PhD obtained in June 2007), and Clément Touya.

Funding: since 2007, the PhyStat group has been funded by one *ANR contract NANO (SIMONANOMEM; coordinator)*, one *European contract (NANOBORON; minority partner)*, one *Appel d'Offres du Conseil Scientifique de l'UPS*, one CNRS grant *Interface physique, biologie et chimie : soutien à la prise de risque*, one CEA grant *contrat Équipe (CENEC)*, and one fellowship from the *Institut Universitaire de France (IUF)*. The PhyStat group currently has two postdoctoral fellowships funded respectively by ANR and CNRS. In addition, PhD fellowships have been awarded by the doctoral school *Sciences de la Matière* and the doctoral school *Biologie – Santé – Biotechnologies* of the University of Toulouse, and by the *Délégation Générale pour l'Armement* (DGA). Like the three other groups, the PhyStat group is also funded by the LPT from its own resources (computers, travel expenses...).

Main visitors: prominent scientists who have visited the PhyStat group for a period of at least one month since 2007 include Prof. Alan J. Bray (Manchester U., UK), Ron R. Horgan (Cambridge U., UK), Paul Krapivsky (Boston U., USA), David Lancaster (Westminster U., UK), Roland R. Netz (TU Munich, Germany), and Sidney Redner (Boston U., USA). They were funded by visiting professor fellowships from the University of Toulouse, CNRS guest scientist fellowships, or by means of the IUF grant.

Insert 1.1 : *Funding of the PhyStat group and its main foreign visitors.*

In addition, the PhyStat group typically hosts one or two Master students per year, during their three-month research projects.

The PhyStat group has several ongoing collaborations with scientific institutions

❍ **In Toulouse:** Institut de Pharmacologie et Biologie Structurale (IPBS; 2 independent collaborations), Institut de Mathématiques de Toulouse (IMT), Laboratoire de Microbiologie et Génétique Moléculaires (LMGM), Observatoire Midi-Pyrénées (OMP).

❍ **In France:** CEA-Saclay, ENS Lyon, ENS Paris, Université de Marseille, Université de Montpellier, Université Paris-Sud Orsay, Université Paris VI Pierre et Marie Curie, Université de Rennes.

❍ **Abroad:** Max Planck Institut – Stuttgart, Technische Universität München (Germany), Synchrotron Trieste, Università di Firenze, Università di Padova, Università di Roma "La Sapienza" (Italy), University of Osaka (Japan), Faculté des Sciences d'Agadir (Morocco), University of Ljubljana (Slovenia), École Nationale d'Ingénieurs de Tunis (Tunisia), London Research Institute, University of Cambridge, University of Manchester, University of Oxford, University of Sheffield, University of Westminster (UK), Carnegie Mellon University, National Health Institute – Bethesda, University of Boston, University of California – Merced, University of California – Santa Barbara (USA).

Insert 1.2 : *Main ongoing collaborations with institutions in Toulouse, France, and abroad (only the hosting university is cited in the two last cases).*

The main sources of funding of the PhyStat group and our medium-term foreign visitors are listed in Insert 1.1. The PhyStat group has ongoing collaborations with many local, French, or foreign institutions, which are listed in Insert 1.2.

D. S. Dean is a current fellow of the *Institut Universitaire de France (IUF; 2007-2012)*, and two members of the PhyStat group have received the Bronze Medal of CNRS in the past (C. Sire in 1994; P. H. Chavanis in 2000; both in section 02 – theoretical physics).

During the last four years, the PhyStat group has published more than **120 articles in refereed international journals** and has contributed to more than **50 conferences (32 invited talks)**. The main aspects of the scientific activity of the PhyStat group during the period 2007-2009 are highlighted in the next three sections. More details can be found on the personal web pages of the members of the PhyStat group.

1.1 Biophysics and soft condensed matter

Despite the inherent complexity of many soft matter, biomimetic, and biological systems (due to interactions $\sim k_BT$, thus large fluctuations, and strong correlations), a deeper fundamental understanding of the physical mechanisms at play could lead to potentially huge payoffs. Areas as important as human health and the worldwide supply of abundant clean water could benefit in the long term from far-reaching advances in comprehension obtained by applying the tools of Statistical Physics to such systems. In this section, we present recent work carried out at LPT PhyStat group, at the interface between physics and biology. This work has already provided greater insight into the thermal denaturation of DNA, the cluster phases of membrane proteins, electropermeabilization of membranes, fluctuation induced interactions in lipid membranes, and ion transport in nanopores.

DNA melting transition

M. Manghi, J. Palmeri, N. Destainville

The thermal denaturation of double-stranded DNA is a physical process in the course of which the double strand, or helix, can open locally thanks to thermal fluctuations that create an opening of successive base pairs, called a denaturation bubble. In the literature, DNA is essentially modeled as a one-dimensional system whose denaturation is described by a 1D Ising model in a "temperature dependent magnetic field" (Poland-Sheraga model) or by an unbinding transition in an orthogonal dimension (Peyrard-Bishop-Dauxois model).

Theory of thermal denaturation of DNA

Recently, J. Palmeri, M. Manghi and N. Destainville [ACL-192] have studied this denaturation process theoretically by illuminating the role of the **coupling between the**

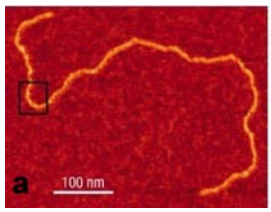
3D non-uniform statistical bending inside a DNA polymer and the **opening and closing of the base pairs** linking the two strands. Within a bubble the two fluctuating single strands are much more flexible than an unopened helix and therefore DNA can explore a much larger number of geometrical configurations when in the bubble state. The DNA geometry will in turn influence the bubble creation process. This mutual influence naturally leads to our coupled theoretical model (Ising-Discrete Worm-like chain model), permitting one to calculate, for example, the denaturation temperature above which the double strand tends to a completely open state (in most previous statistical models, this temperature was put in by hand to analyze experiments). More precisely, the melting temperature is determined by a balance between the energetic cost of opening a base-pair (H-bonds breaking) and the entropic gain in allowing the chain to fluctuate more easily. The statistical properties (end-to-end distance, persistence length) have been calculated as a function of temperature, T, reproducing qualitatively experimental data of DNA solution viscosity measurements. This study has been completed by exploring the influence of the chain length on the melting profile (fraction of open base-pairs *vs* T) [ACL-209, ACL-235] and the role of other chain degrees of freedom such as stretching and torsion [ACL-235].

This work [ACL-192] was recently featured on the scientific news section of CNRS *Institut de Physique* web site.

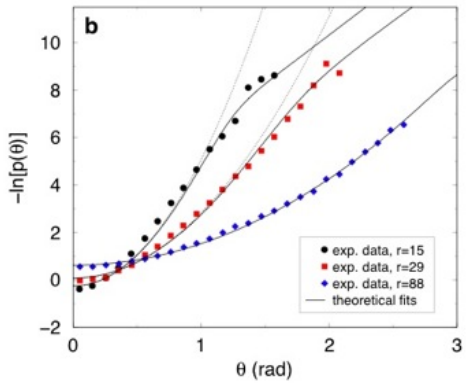
DNA adsorbed on surfaces

Atomic Force Microscopy (AFM) is widely used to observe double-stranded DNA adsorbed on surfaces. In recent experiments by Wiggins *et al.*, "anomalies" have been detected in the distribution of bending angles along DNA $p(\theta)$, which measures its flexibility: an overabundance of large angles was found which is not predicted by the traditional *worm-like chain model* for DNA chains (Insert 1.3). The model has been applied to DNA adsorbed on surfaces by N. Destainville, M. Manghi and J. Palmeri [ACL-236], and these anomalies are related to the presence of **small denaturation bubbles** (or **kinks**) facilitated by the presence of the substrate which modifies the electrostatic interactions between DNA base-pairs. They predict that these anomalies exist in 3D but are too weak to be detected and reconcile the apparent discrepancy between observed 2D and 3D elastic properties. Hence, conclusions about 3D properties of DNA (and its companion proteins and enzymes) do not directly follow from 2D experiments by AFM.

Snapshot of a DNA observed by AFM on a mica surface (experiments by Wiggins *et al.* (2006)).



Experimental bending angle distribution (symbols) for three different values of the distance along the chain. It shows a deviation from the Worm Like Chain model (parabola) for large angles which is well fitted by the theory (solid line).



Insert 1.3 : *DNA adsorbed on surfaces*

Cluster phases of membrane proteins

N. Destainville

N. Destainville studies the dynamical organization of assemblies of bio-membrane proteins. A cell contains several thousand of different proteins species that ensure a large variety of functions. To accomplish their task, they must interact with their parters that often lie in the membrane themselves. To account for the rapidity of the response to an external stimulus, it is generally believed that parters must be co-localized in advance in small membrane **micro-domains**, of size $\sim 100\,\mathrm{nm}$. To explain this compartmentalization, two models are usually invoked: lipid rafts, resulting from a lipidic micro-phase separation, and the

"fence-and-picket model" for non-raft proteins, which supposes the delimitation of membrane domains by actin filaments of the cytoskeleton. In this context, N. Destainville proposed a new paradigm explaining the existence of micro-domains, based upon an **analogy with cluster phases in colloidal physics**. The coexistence of effective short-range attractive forces and longer-range repulsive ones ensures the existence, at equilibrium, of proteins clusters of a few tens or hundred of proteins, which play the role of the above-mentioned compartments. The interactions taken into account are mediated by the lipidic membrane in which the proteins dwell, and are on the order of the thermal energy k_BT.

These cluster phases have been studied by numerical [ACL-211] as well as analytical [ACL-212] means. It has been shown that the mean-cluster size grows proportionally to the protein concentration ϕ and that the mean diffusion coefficient of proteins is inversely proportional to ϕ. These results have been discussed in the context of biological membranes in the review article [ACL-214]. Work is in progress to study the role of the great diversity of membrane proteins and to test these predictions at the experimental level, in collaboration with the group of L. Salomé at the Institut de Pharmacologie et Biologie Structurale (Toulouse).

Electropermeabilization

D. S. Dean, T. Portet

Electropermeabilization is the phenomenon via which biological membranes are rendered permeable to the passage of molecules and even macro-molecules by the application of an electric field [ACL-185, ACL-189, ACL-231, ACL-234, SRP-11]. This effect is extensively exploited in medicine, specifically in the field of cancer and genetic therapy. In chemotherapy, the permeabilizing effect of the electric field enables the treatment of cancers in a much more targeted way (only the region of the tumor is subjected to the field) and the enhanced permeability due to the electric field means that much lower doses of chemotherapeutic drugs can be administered, greatly reducing side effects. Electropermeabilization is also a promising candidate for gene therapy treatments and does not entail the same risks as viral mediated gene transfer [ACL-185, ACL-231]. The PhyStat group has launched a collaboration with the team of M.-P. Rols at the IPBS Toulouse, one of the world leading experimental groups in the field. Currently, a PhD student (T. Portet) is being co-supervised by D. S. Dean and M.-P. Rols.

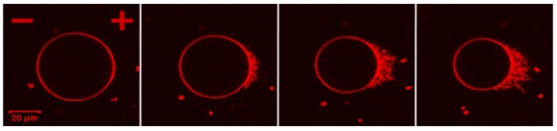


Figure 1.1 : *Confocal images of a lipid giant unilamellar vesicle subjected to electric pulses (360 V/cm; 0.5 Hz; 5 ms duration), exhibiting size decrease and the formation of tubular structures facing the anode. 6 pulses are applied between each snapshot.*

We have shown that giant unilamellar vesicles subjected to electropermeabilizing pulses tend to shrink [ACL-234]. The vesicles lose lipids from the main body via three mechanisms (i) the formation of pores, (ii) the budding off of micro-vesicles and (iii) the formation of vesicle tubules (see Fig. (1.1). These novel experimental results can be partly explained in a model where we assume lipid loss is proportional to the area where the lysis tension of the lipid membrane is exceeded (due to the addition of that coming from the Maxwell stress tensor of the applied field). We have also been studying the permeabilization of cells in the presence of plasmid DNA (4.7 kb). This problem is of practical importance (gene therapy) and also the underlying physics is rich (permeabilization of the membrane, interaction of DNA with the membrane and the electrophoretic transport of the DNA) [ACL-189]. We have modeled the transport of DNA in the region of a cell which is assumed to have a pore formed by electroporation. The model explains experiments carried out at the IPBS and confirms that the major obstacle to gene transfer is the actin cytoskeleton of the cell interior [SRP-11].

Fluctuation induced interactions

D. S. Dean, M. Manghi

Pseudo Casimir effects arise via the thermal fluctuations of classical fields such as those

describing the order parameter of classical systems near critical points, the director fluctuations in liquid crystals and the height fluctuations of lipid membranes. We have studied the effective interactions between regions of lipid membranes of varying elasticity and bending rigidity. In [ACL-170] we showed that regions of differing mechanical properties (due to differing lipid types) could have attractive or repulsive interactions between them, meaning that the nature of the phase transition in membranes formed from lipid mixtures could be drastically modified by membrane height fluctuations. A thermal Casimir effect between large striped membrane regions of differing mechanical properties was demonstrated in [ACL-190].

In soft matter systems, where relaxation times can be large, it makes sense to ask how the Casimir force evolves out of equilibrium. To study this problem we considered a formulation of the Casimir effect where the energy of interaction of the fluctuating field with the boundaries or objects placed in the field is specified [ACL-232]. We were able to study the effect of these soft boundary conditions on systems of two and even three parallel plates. In the case of soft boundary conditions, whether or not the fluctuations exist outside the two external plates drastically affects the force on the central plate and can even change its sign. In [ACL-245], using this boundary energy formalism, we were able to compute the force on objects and surfaces in fluctuating fields out of equilibrium for a very general class of dissipative dynamics. In [ACL-242] the thermal Casimir or zero frequency van der Waals interaction between slabs of random dielectric media was studied. This calculation represents the first ever analysis of the Casimir effect in disordered systems. Two important physical points were found: (i) the long range force is self-averaging and is given by a description in terms of effective dielectric constants; (ii) the short range force is a random variable, dominated by the closest opposing layers.

Ion partitioning and transport in nanoporous membranes

J. Palmeri, M. Manghi, D. S. Dean, L. Horvath (PhD student), S. Buyukdagli (postdoc)

Using macroscopic mean field, field theoretic, and microscopic molecular dynamical (MD) simulation methods, our goal is to better understand the physical and physicochemical phenomena involved in nano-confined aqueous solutions, especially the role of "solute-solute" and "solute-interface" interactions in nanofiltration [ACL-140, ACL-193, COD-3, ACL-142]. We focus on effects due to the specific characteristics of molecules and ions (size, charge, polarizability) by studying their distribution, correlations, and fluctuations near interfaces and in nanopores [TH-14, TH-15, ACTI-20, AFF-30].

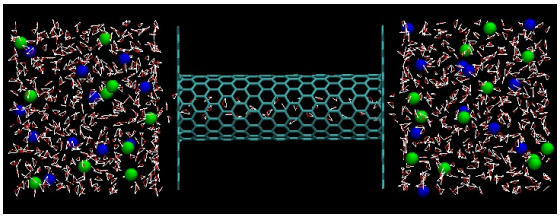


Figure 1.2 : *MD Snapshot of a nanopore with 1M Na Cl in water [TH-15].*

1.2 Stochastic processes and disordered systems

Many systems in Nature can be well described by effective random processes. From the diffusing trajectories of dust particles or proteins on the cell membrane (see Section 1.1), to financial signals, statistical physics has developed efficient tools to model a large class of physical, biological, or social signals, thereby giving a better qualitative and quantitative understanding of extremely complex systems. In the present section, we review a series of recent fundamental results obtained at LPT in the field of stochastic processes and disordered systems, and illustrate some of their applications.

Persistence and extreme value statistics

D. S. Dean, C. Sire

The persistence $P(M,t)$ of a general temporal signal $x(t)$ is the probability that this signal always remains above (or below) a certain threshold M from time 0 up to time t. In the period 1996-2001, C. Sire, S. N. Majumdar (CR1 at LPT in 1999-2004, now DR2 at LPTMS Orsay), and their collaborators in Manchester and Jülich developed powerful methods to evaluate the large

time asymptotics of the persistence (and hence the persistence exponent) for physically relevant signals, but **only** when M is equal to the mean of x. Persistence exponents have been measured in systems as different as breath figures, liquid crystals, laser-polarized Xe gas, fluctuating steps on a Si surface, and soap bubbles. The aforementioned theories are in very good agreement with experiments (and numerical simulations) in all these cases. The two following studies illustrate the deep connection between **persistence and extreme value statistics**.

General theory of persistence

Recently [ACL-195, ACL-223], C. Sire has obtained a very precise approximation for $P(M,t)$, for arbitrary M and t, from the sole knowledge of the two-time correlation function of the random process x (not necessarily Gaussian). This theory gives access to the distribution of the minimum (or the maximum) of a general signal during a time window of duration t, since $P(M,t)$ is exactly the probability that the minimum of x over the interval $[0,t]$ be larger than M. Many general results have been obtained [ACL-223] for the distribution of time intervals at which the signal crosses the threshold M, and the approximation of [ACL-195] either reproduces most of these exact results, or turns out to be an excellent approximation.

Random matrices and persistence

As an original example of persistence, D. S. Dean and S. N. Majumdar computed exactly the probability that an $N\times N$ Gaussian Hermitian/real symmetric random matrix has all its eigenvalues above a certain threshold M [ACL-167, ACL-216]. This persistence probability decays exponentially with the number of entries N^2, and the rate is exactly the persistent exponent. Generalizing the celebrated Wigner semi-circle law, they obtained the corresponding conditional density of states of the eigenvalues, in the large N limit.

Theory of competition

C. Sire, D. S. Dean

Physicists are now more then ever involved in the study of complex systems which do not belong to the traditional realm of their science. Finance (option pricing theory,...), human networks (Internet, airports,...), the dynamics of biological evolution and in general of competitive "agents" are just a few examples of problems recently addressed by statistical physicists. In this section, four recent studies concerning **the theory of competition** are summarized. All are intimately related to the persistence problem, extreme value statistics, and traveling wave theory.

The "leader" problem

C. Sire, D. S. Dean, and S. N. Majumdar have defined a very general kind of competition which arise as a simplification of some evolutionary biology models. N "agents" have random fitnesses v_i, and obtain a "score" $s_i(t) = s_i(0) + v_i t$ at time t, where the initial scores are random variables. At large enough time, the leader of the pack (the agent with the highest score) will ultimately be the one having initially the largest fitness. A natural question thus arises: **how many different leaders were there during the competition?** In most practical examples of a general finite-time competition (see the case of poker tournaments below), one observes numerically that the total number of leaders behaves like $\log N$, and that the proportionality constant is universal. In [ACL-178], these results have been rigorously and explicitly derived and the authors obtained the full distribution of the number of leaders starting from N players.

Universal dynamics of poker tournaments

Poker tournaments, although *a priori* controlled by purely human factors (fear, bluff...), are a perfect laboratory to test the possible application of statistical physics methods to social systems: contrary to most other challenging systems (finance, social networks, epidemics...), they are **perfectly isolated** from the influence of the outside world.

C. Sire has developed a numerical model which mimics the dynamics of a poker tournament with initially N players [ACL-197]. This model can be analytically solved and its results are in perfect agreement with data gathered from actual Internet tournaments or live World Championships. The average duration of the tournament and the number of successive "chip-leaders" (the player with the biggest fortune at

a given time) are both found to be proportional to $\log N$, in agreement with the general result of [ACL-178]. The distribution of the fortune of the current chip-leader is universal and follows the Gumbel law, well-known in the context of extreme value statistics. The most spectacular result concerns a faithful description of the rank of a player at a given time, as a function of his current fortune, which is illustrated in Fig. 1.3. This work has received important media coverage (Scientific American, PhysOrg.com, and many others).

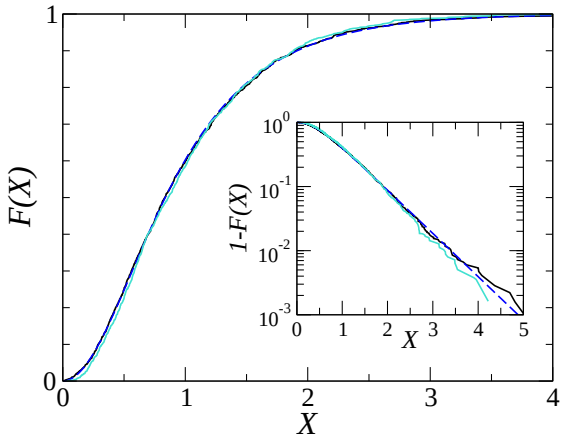


Figure 1.3 : *Plot of the fraction $F(X)$ of players who are poorer than a given player owning X times the average fortune. $F(X)$ does not depend explicitly on time (scale invariance). The solution of the model (blue dashes; no parameter fit) agrees perfectly with data collected from 22 Internet tournaments (black) and the full 2006 season of the Word Poker Tour (light blue).*

Baseball team standings and streaks

C. Sire and S. Redner (Boston) have modeled sport leagues [ACL-241] to quantify the distribution of a team's wins and losses in major-league baseball over the past century, and also to argue that long winning and losing streaks are of purely statistical origin. The data further reveal that the past half-century of baseball has been more competitive than the preceding half-century, and the analysis points to subtle effects due to the finite number of matches in a season.

Contest based on a random polymer

C. Sire has defined and solved a two-player game inspired by a model of a directed polymer on the Cayley tree (the tree of possible moves) [ACL-224]. The fact that the two players have antagonist goals is reminiscent of the notion of **frustration** common in disordered physical systems. The solution involves extreme value statistics and front wave propagation, including a subtle non linear front velocity selection mechanism.

Diffusion in random media

D. S. Dean, C. Sire, J. Sopik (PhD student), and C. Touya (PhD student)

Diffusion in random media is an interesting subject in its own right and also because systems exhibiting structural glass transitions often behave like systems with quenched disorder (which is dynamically induced). Other applications are to theories of absorption/growth processes (like DLA), where renormalization group techniques developed for diffusion in random media have been successfully adapted [ACL-177].

Diffusion in non-Gaussian random potentials

In the past, there have been many studies of the diffusion of a particle in a short range Gaussian potential ϕ. In finite dimensions, the diffusion constant of the particle is always non-zero at finite temperatures and no transition between a normal and sub-diffusive regime can occur. However, for a potential which is a function of a Gaussian potential $V = V(\phi)$, a transition can occur and this transition can be identified as the divergence of the mean occupation time in local minima [ACL-194]. An example is the potential $V(\phi) = \phi^2/2$, which physically arises when one considers dipoles in a random Gaussian electric field [ACL-246]. This model in dimension $D = 1$ and a particular variant in $D = 2$ can be treated analytically. The effective diffusion constant vanishes as $\kappa_e \sim (1 - \beta^2)^{\frac{1}{2}}$ ($\beta = 1/k_B T$), in a way reminiscent of that predicted by mode-coupling theories of the glass transition. The low temperature exponent characterizing the sub-diffusion was also computed using a version of the replica method applied to the first-passage time problem. In higher dimensions, analytic results are not available and one must resort to approximation schemes. A self-similar renormalization

group approach [ACL-217] was applied to the mathematically related problem of diffusion in a medium of random diffusivity, where the diffusion equation has the form $\dot{p} = \nabla \cdot \kappa(\mathbf{x}) \nabla p$. If one assumes that $\kappa = \kappa(\phi(\mathbf{x}))$ where ϕ is Gaussian, the self similar RG yields the result:

$$\kappa_e^{(p)} = \left\langle \kappa(\mathbf{x})^{1-\frac{2}{D}} \right\rangle^{\frac{1}{\left(1-\frac{2}{D}\right)}} \tag{1.1}$$

This result is a widely used approximation in the field of effective permeabilities (for random dielectrics and porous media) and this form is sometimes referred to as the Landau-Lifshitz-Matheron conjecture. From Eq. (1.1), using a mathematical relation between the two problems, we computed the effective diffusion constant for diffusion in a random potential $V(\phi)$. For quadratic V, this result gives the celebrated Volger-Fulcher-Tammann divergence of the relaxation time $\tau \sim 1/\kappa_e$ as one approaches the glass transition. A final result of this analysis concerns a tentative link with the diffusion constant of interacting Langevin particles. The potential seen by a particle is the sum over the pairwise interactions. Treating this potential as effectively random, the self-similar RG predicts the self-diffusion constant of the particles to be $\kappa_e = \exp(2\beta s_{ex}/D)$, where s_{ex} is the excess entropy. This sort of result has been observed in the literature on molecular dynamics simulations, but has not been understood theoretically.

Average number of critical points of Gaussian random fields

Gaussian random fields are of particular importance, as they can be argued to occur spontaneously in systems with a large number of degrees of freedom by appealing to the central limit theorem. The study of the distribution of critical points of complex and random fields occurs in a number of physical problems ranging from string theory (where the local minima of the string landscape correspond to possible universes), theories of the structural glass and spin glass transition (the onset of the glass transition is often identified with the point where the critical points in the free energy landscape become dominated by minima), theoretical studies of hard optimization problems and the problem of protein folding. In [ACL-186], we were able to compute the average number of critical points of a Gaussian potential, on a high dimensional space, at fixed value of the potential and at fixed number of negative eigenvalues at the critical point. This work presents a significant technical advance as the only previous results which existed were for the total average number of critical points and for the average number of local minima.

1.3 Statistical physics of systems with long range interactions

Systems with long-range interactions are numerous in nature and present the remarkable property of self-organizing spontaneously into coherent structures. This corresponds to galaxies in astrophysics (stellar systems), large scale vortices in geophysical and astrophysical flows (two-dimensional turbulence), aggregates of bacteria in biology (chemotaxis), and clusters in the HMF toy model. Interestingly, it is possible to understand the structure and organization of these very different systems in terms of similar arguments of statistical mechanics and kinetic theory.

The Hamiltonian Mean Field (HMF) model

P. H. Chavanis, L. Delfini (postdoc)

The HMF model describes the evolution of N rotators coupled through an attractive cosine interaction. The Hamiltonian reads

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{N} p_j^2 + \frac{1}{2}\sum_{i,j=1}^{N}[1-\cos(\theta_i - \theta_j)], \tag{1.2}$$

where θ_i represents the orientation of the i-th rotator and p_i stands for the conjugated momentum. To monitor the evolution of the system, it is customary to introduce the magnetization, an order parameter defined as $M = |\sum_i \mathbf{m}_i|/N$, where $\mathbf{m}_i = (\cos\theta_i, \sin\theta_i)$.

For $t \to +\infty$, this system is expected to reach a statistical equilibrium state described by the Boltzmann distribution. However, numerical simulations of the N-body system show a more complex behavior (see Fig. 1.4 from [ACL-230]). Indeed, the system **gets stuck in a quasi-stationary state (QSS) that differs from the Boltzmann distribution**. This discovery was a surprise in the statistical mechanics community and different approaches such as the generalized thermodynamics of Tsallis have been

proposed to account for these QSS. In fact, the same phenomenon was previously observed in self-gravitating systems and 2D turbulence where an explanation in terms of a statistical mechanics of the Vlasov equation was proposed a long-time ago by D. Lynden-Bell [1]. This approach was not well-known by the statistical mechanics community and P. H. Chavanis [ACL-158] has contributed to popularizing it.

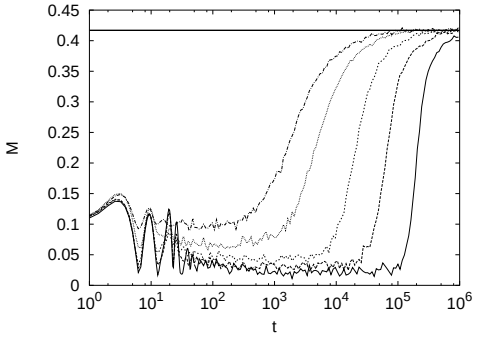


Figure 1.4 : *Evolution of the magnetization $M(t)$ for different values of the particle number N [ACL-230]. For $t \to +\infty$, the system relaxes towards the Boltzmann distribution (solid line). However, before reaching this statistical equilibrium state, it remains frozen in a QSS (plateau), whose lifetime diverges as $N \to +\infty$.*

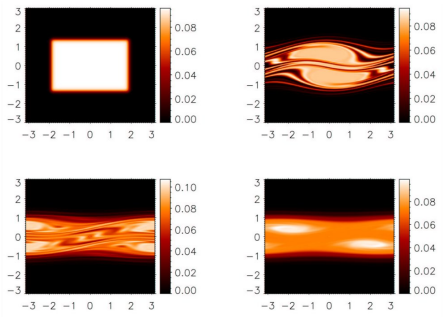


Figure 1.5 : *Numerical simulation of the Vlasov equation in phase space starting from an initial distribution function $f(\theta, v, t = 0)$ taking only two values $f = f_0$ or $f = 0$ [ACTI-24]. This figure reveals the complicated mixing process leading to a QSS on a coarse-grained scale, corresponding to violent collisionless relaxation.*

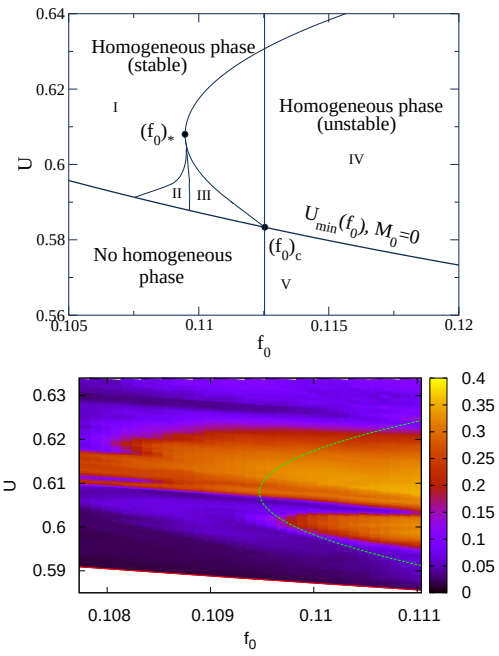
Using the Lynden-Bell theory of **violent relaxation** (see Fig. 1.5), P. H. Chavanis and his colleagues [ACL-158, ACL-180, ACTI-24, ACL-230] have determined the out-of-equilibrium phase diagram of the HMF model (see Insert 1.4). The prediction depends on two control parameters: the energy U and the value f_0 of the initial distribution function. Varying these parameters, an out-of-equilibrium phase transition occurs [ACL-158, ACL-180], where the QSS can be either un-magnetized (the system of rotators is spatially homogeneous) or magnetized ($M \neq 0$; inhomogeneous). A more detailed analysis [ACTI-24, ACL-230] shows that there exists on the same diagram **first and second order phase transitions** that merge at a tricritical point $((f_0)_*, U_*) = (0.10947, 0.608)$. Furthermore, the phase diagram displays an interesting phenomenon of **phase re-entrance** [ACL-158]: if f_0 lies in the small interval $[0.10947, 0.1125]$, by decreasing progressively the energy, the QSS is successively homogeneous, inhomogeneous, and homogeneous again.

Recently, this theoretical prediction has been confronted with direct numerical simulations of the N-body Hamiltonian system [ACL-230]. The phase re-entrance phenomenon is confirmed (see Insert 1.4). This is remarkable because phase re-entrance occurs in a very small range of parameters which would have been difficult to find without the theoretical prediction. The existence of first and second order phase transitions has also been confirmed numerically. However, the simulations show that the picture is more complicated than the prediction of the Lynden-Bell theory. In particular, there exists a secondary zone of phase re-entrance in the magnetized region and a persistence of magnetized states in the un-magnetized region. These anomalies are probably the result of an *incomplete relaxation* as observed in other domains [ACL-149], but it is difficult to make predictions when the evolution of the system is non-ergodic.

On longer timescales, the system is expected to converge towards the Boltzmann distribution due to correlation/finite N effects ("collisions"). P. H. Chavanis and his colleagues [ACL-206] have investigated numerically this phase of slow

1. D. Lynden-Bell, Mon. Not. R. Astron. Soc. **136**, 101 (1967).

collisional relaxation. They have found that, in the collisional regime, the distribution function $f(\theta, p, t)$ is well-fitted by q-Gaussian distributions (Tsallis distributions) with an index $q(t)$ evolving in time. When the $q(t)$-parameter reaches a critical value $q_c(U)$, the distribution becomes Vlasov unstable [ACL-206, ACL-244] [2] and a dynamical phase transition takes place which rapidly drives the system towards the Boltzmann distribution. This corresponds to the sudden transition from the non-magnetized QSS to the magnetized equilibrium state that can be observed on Fig. 1.4.



Out-of-equilibrium phase diagram of the HMF model in the framework of Lynden-Bell's theory of violent relaxation [ACL-158, ACTI-24] (top), and as obtained from direct numerical simulations (bottom), which confirms the main theoretical predictions (phase re-entrance, first and second order phase transitions...).

Insert 1.4 : *Theoretical and numerical phase diagram of the HMF model.*

Thermodynamics of self-gravitating Brownian particles and chemotaxis of bacterial populations

P. H. Chavanis, C. Sire, J. Sopik (PhD student)

In biology, many organisms (bacteria, amoebae, cells,...) or social insects (ants, swarms,...) interact through the process of chemotaxis. Chemotaxis is a long-range interaction that accounts for the morphogenesis and self-organization of biological systems. A first successful model of chemotactic aggregation is provided by the Keller-Segel (KS) model [3]:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D_* \nabla \rho - \chi \rho \nabla c), \qquad (1.3)$$

$$\frac{\partial c}{\partial t} = D_c \Delta c - kc + h\rho. \qquad (1.4)$$

It consists in two coupled differential equations that govern the evolution of the density of cells (or other biological entities) $\rho(\mathbf{r}, t)$ and the evolution of the secreted chemical $c(\mathbf{r}, t)$. Eq. 1.3 is a drift-diffusion equation. The cells diffuse with a diffusion coefficient D_* and they also move in a direction of a gradient of the chemical (chemotactic drift). The second equation Eq. 1.4 in the KS model is a reaction-diffusion equation. The chemical is produced by the bacteria with a rate h and is degraded with a rate k. It also diffuses with a diffusion coefficient D_c. When chemotactic attraction prevails over diffusion, the KS model describes a *chemotactic collapse* leading to aggregates or Dirac peaks (see Fig. 1.6).

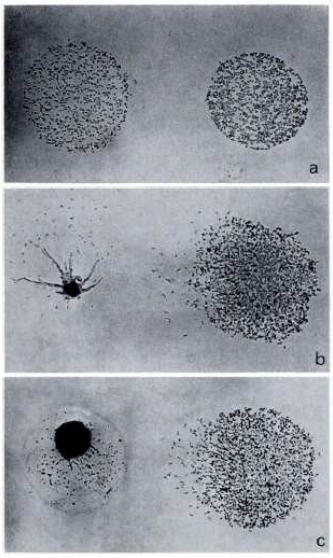


Figure 1.6 : *An experimental example of chemotactic collapse.*

The first equation of the KS model can be

2. [ACL-244] was recently highlighted in *Europhysics News* **40**, 13 (2009).
3. E. Keller and L. A. Segel, J. Theor. Biol. **26**, 399 (1970).

interpreted as a mean field Smoluchowski equation describing a system of Brownian particles in interaction. On the other hand, in the limit of large diffusivity of the chemical, and when the degradation of the chemical can be neglected, the second equation reduces to a Poisson equation $D_c\Delta c = -h\rho$. In that case, we find that the simplified KS model becomes equivalent to the Smoluchowski-Poisson (SP) system

$$\frac{\partial\rho}{\partial t} = \nabla\cdot\left[\frac{1}{\xi}\left(\frac{k_BT}{m}\nabla\rho+\rho\nabla\Phi\right)\right], \quad (1.5)$$

$$\Delta\Phi = G\rho, \quad (1.6)$$

describing a system of overdamped self-gravitating Brownian particles in the mean field approximation. We have the correspondence: $D_* = k_BT/\xi m$, $\chi = 1/\xi$, $c = -\Phi$, $\lambda = G$. In particular, the **concentration of the secreted chemical** $c(\mathbf{r},t) = -\Phi(\mathbf{r},t)$ in biology plays the role of the **gravitational potential** (with the opposite sign) in astrophysics.

P. H. Chavanis and C. Sire [ACL-157, ACL-159, ACL-182, ACL-183, ACL-174, ACL-175, ACL-196, ACL-220, ACL-222] have performed a detailed analytical and numerical study of these equations. The extension of these studies to a multi-species system has been done with J. Sopik [ACL-143]. The theoretical problem is very rich because several regimes can occur depending on the value of the temperature, the dimension of space and whether the system is in a bounded or an unbounded domain. Typically, three types of evolution are possible: (i) convergence towards an equilibrium state for $t\to+\infty$. (ii) collapse in finite or infinite time. (iii) evaporation. P. H. Chavanis and C. Sire have performed a detailed study of the equilibrium phase diagram in order to determine under which conditions the system can achieve an equilibrium state. When no equilibrium state exists, the system can either collapse or evaporate. In that case, the strategy is to look for self-similar solutions describing the evolution of the system. Despite the mathematical complexity of the problem, it has been possible to provide analytical solutions for all the phases of the dynamics. In particular, in two dimensions, it is possible to compute exactly (*i.e.* for any particle number N) the diffusion coefficient of self-gravitating Brownian particles [ACL-174, ACL-183]:

$$D(T) = \frac{k_BT}{\xi m}\left(1-\frac{T_c}{T}\right), \quad (1.7)$$

involving the critical temperature

$$k_BT_c = (N-1)\frac{Gm^2}{4}. \quad (1.8)$$

The classical Einstein relation is recovered for $G = T_c = 0$. This expression shows that the system evaporates for $T > T_c$ and undergoes a finite time collapse for $T < T_c$.

P. H. Chavanis and C. Sire have also developed a kinetic theory of chemotaxis leading to hydrodynamic equations including a friction force [ACL-198, ACL-156, ACL-221]. The KS model is recovered in the limit of strong friction and leads to point wise blow-up. Alternatively, when the friction coefficient is reduced, the aggregates are replaced by a filamentary structure. These filaments are observed in experiments of blood vessel formation and they have been proposed to explain vasculogenesis. They are also observed in cosmology, where the evolution can be described by the Euler-Poisson system.

Other works

P. H. Chavanis

P. H. Chavanis has developed other aspects of the dynamics and thermodynamics of systems with long-range interactions. He studied the lifetime of metastable states of self-gravitating systems (such as globular clusters) and showed that it scales like e^N, with $N\sim 10^6$. Therefore, even if these systems are only local entropy maxima, they are very robust in practice [ACL-127]. Extending the Chandrasekhar theory of relativistic white dwarf stars in d dimensions, he showed that white dwarf stars become unstable in a space of dimension $d\geq 4$ [ACL-181]. He also developed an analogy between relativistic stars with a linear equation of state and black holes, and discovered a critical dimension $d_c = 9.96404372...$ for self-gravitating radiation (photon stars) in general relativity [ACL-203]. With F. Bouchet, he described the evolution of collisionless stellar systems on the coarse-grained scale [ACL-128]. With B. Dubrulle *et al.*, he developed the statistical mechanics of 3D axisymmetric magnetohydrodynamics and granular flows [ACL-128, ACL-148, ACL-243]. With M. Lemou, he developed the kinetic theory of point vortices [ACL-184, ACL-201].

2

Scientific production of the PhySTAT group (2005-2009)

The PhySTAT group addresses a large variety of problems using the analytical and numerical tools of statistical physics, and in particular, out of equilibrium physics. During the last ten years, it has developed a strong activity in the field of soft condensed matter physics (ionic fluids, polymers, lipidic films, porous media...) and biophysics (cell membrane, DNA, biological engines,...), collaborating and sharing contracts with several experimental groups of biologists and physicists. The PhySTAT group has also a strong expertise in the applications of stochastic processes in various contexts (diffusing processes in random media, theory of signals, theory of competition, optimisation problems...), and the physics of long-range interacting systems (with applications to turbulence, astrophysics, chemotaxis...). We list the *full* scientific production of the PhySTAT group during the period 2005-2009. The diversity of subjects treated in the PhySTAT group translates into an equally large variety of scientific journals and conferences where its six permanent scientists publish or present their works.

Following the AERES recommendation, the scientific production of the PhySTAT group is listed according to the following categories:

- **Articles published in refereed journals** (ACL; page 18): **121**
- **Articles without reference (preprints)** (SRP; page 23): **4**
- **Invited talks in international and national conferences** (INV; page 24): **32**
- **Oral communications with a conference proceeding (international conferences)** (ACTI; page 25): **9**
- **Oral communications not leading to a conference proceeding** (COM; page 26): **11**
- **Posters in conferences** (AFF; page 26): **9**
- **Books or book chapters** (OS; page 27): **1**
- **Vulgarization publications** (OV; page 27): **7**
- **Books as Editor** (DO; page 27): **1**
- **Commercial and Open Source softwares** (COD; page 28): **1**
- **Habilitation thesis to supervise researches** (HDR; page 28): **1**
- **PhD thesis completed or in progess** (TH; page 28): **8**

Some statistical data on LPT refereed publications:

❍ The **average number of authors** on a LPT ACL/SRP publication is just below 3: 1.3 permanent researcher at LPT, 0.25 postdoc or PhD student at LPT (excluding LPT visitors), 1.4 non LPT researcher (including LPT visitors) [1]. LPT permanent researchers are underlined and LPT postdocs/PhD students are dash-underlined in the publication list below.

❍ Since 2005, around **250 authors** have participated to LPT publications (including LPT permanent staff, postdocs, and PhD students at LPT). They work in more than **120 different institutions outside Toulouse** [2] and **6 laboratories on UPS campus** [3].

❍ Percentage of LPT publications since 2005 having **at least one author from a foreign institution [2] (21 countries)**: Germany 20 %, Switzerland 8 %, USA 7.5 %, UK 6 %, Italy & Russia 4.5 %, Canada & Japan & Poland 2 %...

❍ The roughly **1000 publications** of the 18 active permanent researchers presently working at LPT have gathered around **17000** citations and 90/45 articles have received more than 50/80 citations (mean – and median – age of LPT active researchers as on 1st January 2010: 42) [4].

The references in light green are linked to their ArXiv preprint in *pdf* or to the corresponding journal web site (subscription needed in this case), and can thus be directly consulted from the *pdf* version of the present document. Most LPT publications since 2006 are also referenced on CNRS HAL repository.

2.1 Articles published in refereed journals

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[ACL-128] P. H. Chavanis and F. Bouchet, *On the coarse-grained evolution of collisionless stellar systems*, *Astronomy and Astrophysics* **430**, 771 (2005).

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1. FFC: 1.3/0.33/2.1; Quantware: 1.3/0.33/0.8; PhyStat: 1.2/0.11/1.1; Agrégats: 1.6/0.37/2.4. Publications of LPT groups heavily involved in numerical simulations logically involve more authors.

2. Analyzing search results on ISI Web of Sciences.

3. Institut de Pharmacologie et Biologie Structurale (2 independent collaborations), Institut de Mathématiques de Toulouse, Laboratoire de Microbiologie et Génétique Moléculaires, Laboratoire de Chimie et Physique Quantiques, Laboratoire National des Champs Magnétiques Intenses, Observatoire Midi-Pyrénées.

4. Rough estimates obtained from ISI Web of Sciences based on LPT scientists individual records and estimating overlaps. LPT publications are systematically signed under the affiliation Laboratoire de Physique Théorique since 2004 only.

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[ACL-204] P. H. Chavanis, *Hamiltonian and Brownian systems with long-range interactions: V. Stochastic kinetic equations and theory of fluctuations*, Physica A **387**, 5716 (2008).

[ACL-205] P. H. Chavanis, *Statistical mechanics of 2D turbulence with a prior vorticity distribution*, Physica D **237**, 1998 (2008).

[ACL-206] A. Campa, P. H. Chavanis, A. Giansanti, and G. Morelli, *Dynamical phase transitions in Hamiltonian long-range systems and Tsallis distributions with time dependent index*, Physical Review E **78**, 040102(R) (2008).

[ACL-207] P. H. Chavanis, *Two-dimensional Brownian vortices*, Physica A **387**, 6917 (2008).

[ACL-208] R. Monchaux, P. H. Chavanis, A. Chiffaudel, P. P. Cortet, F. Daviaud, P. Diribarne, and B. Dubrulle, *Fluctuation-Dissipation Relations and statistical temperatures in a turbulent von Karman flow*, Physical Review Letters **101**, 174502 (2008).

[ACL-209] J. Palmeri, M. Manghi, and N. Destainville, *Thermal denaturation of fluctuating finite DNA chains: The role of bending rigidity in bubble nucleation*, Physical Review E **77**, 011913 (2008).

[ACL-210] N. Destainville, *Theory of fluorescence correlation spectroscopy at variable observation area for two-dimensional diffusion on a meshgrid*, Soft Matter **4**, 1288 (2008).

[ACL-211] N. Destainville, *Cluster phases of membrane proteins*, Physical Review E **77**, 011905 (2008).

[ACL-212] N. Destainville and L. Foret, *Thermodynamics of nano-cluster phases: a unifying theory*, Physical Review E **77**, 051403 (2008).

[ACL-213] N. Destainville, A. Saulière, and L. Salomé, *Comment to the paper of Michael J. Saxton: "A Biological Interpretation of Transient Anomalous Subdiffusion. I. Qualitative Model"*, Biophysical Journal **95**, 3117 (2008).

[ACL-214] N. Destainville, F. Dumas, and L. Salomé, *What do diffusion measurements tell us about membrane compartmentalization? Emergence of the role of interprotein interactions*, Journal of Chemical Biology **1**, 37 (2008).

[ACL-215] N. Destainville and V. Desoutter, *Slow flip dynamics of three-dimensional rhombus tilings: failure of the Langevin approach*, Applied Mathematics & Information Sciences **2**, 83 (2008).

[ACL-216] D. S. Dean and S. N. Majumdar, *Extreme value statistics of eigenvalues of Gaussian random matrices*, Physical Review E **77**, 041108 (2008).

[ACL-217] D. S. Dean and C. Touya, *Self similar renormalization group applied to diffusion in non-Gaussian potentials*, Journal of Physics A **41**, 335002 (2008).

[ACL-218] M. Manghi and M. Aubouy, *Adsorption of polyelectrolytes from semidilute solutions on an oppositely charged surface*, Physical Chemistry Chemical Physics **10**, 1697 (2008).

[ACL-219] S. Touil, J. Palmeri, S. Tingry, S. Bouchtalla, and A. Deratani, *Generalized dual mode modeling of xylene isomer sorption in polyvinylalcohol membranes containing alpha cyclodextrin*, Journal of Membrane Science **317**, 2 (2008).

[ACL-220] P. H. Chavanis and C. Sire, *Critical mass of bacterial populations in a generalized Keller-Segel model: Analogy with the Chandrasekhar limiting mass of white dwarf stars*, Physica A **387**, 1999 (2008).

[ACL-221] P. H. Chavanis and C. Sire, *Jeans type analysis of chemotactic collapse*, Physica A **387**, 4033 (2008).

[ACL-222] C. Sire and P. H. Chavanis, *Critical dynamics of self-gravitating Langevin particles and bacterial populations*, Physical Review E **78**, 061111 (2008).

[ACL-223] C. Sire, *Crossing intervals of non-Markovian Gaussian processes*, Physical Review E **78**, 011121 (2008).

[ACL-224] C. Sire, *Contest based on a directed polymer in a random medium*, Physical Review E **78**, 061106 (2008).

[ACL-225] F. Baldovin, P. H. Chavanis, and E. Orlandini, *Microcanonical quasi-stationarity of long-range interacting systems in contact with a heat bath*, Physical Review E **79**, 011102 (2009).

[ACL-226] P. H. Chavanis, *Dynamical and thermodynamical stability of two-dimensional flows : variational principles and relaxation equations*, European Physical Journal B **70**, 73 (2009).

[ACL-227] P. H. Chavanis, *Kinetic theory of stellar systems, two-dimensional vortices and HMF model*, Theoretical and Computational Fluid Dynamics, in press (2009).

[ACL-228] P. H. Chavanis, *A stochastic Keller-Segel model of chemotaxis*, Communications in Nonlinear Science and Numerical Simulation **15**, 60 (2010).

[ACL-229] P. H. Chavanis, *Statistics of the gravitational force in various dimensions of space: from Gaussian to Lévy laws*, European Physical Journal B **70**, 413 (2009).

[ACL-230] F. Staniscia, P. H. Chavanis, G. De Ninno and D. Fanelli, *Out-of-equilibrium phase re-entrance(s) in long-range interacting systems*, Physical Review E **80**, 021138 (2009).

[ACL-231] J.-M. Escoffre, T. Portet, L. Wasungu, J. Tessié, D. S. Dean and M.-P. Rols, *What is (still not) known of the mechanism by which electroporation mediates gene transfer and expression in cells and tissues*, Molecular Biotechnology **41**, 286 (2009).

[ACL-232] D. S. Dean, *Thermal Casimir effect with soft boundary conditions*, Physical Review E **79**, 011108 (2009).

[ACL-233] D. S. Dean, R. R. Horgan, A. Naji, and R. Podgornik, *One-dimensional counterion gas between charged surfaces: Exact results compared with weak- and strong-coupling analysis*, Journal of Chemical Physics **130**, 094504 (2009).

[ACL-234] T. Portet, F. Camps, I. Febrer, J.-M. Escoffre, C. Favard, M.-P. Rols, and D. S. Dean, *Visualization of lipid expulsion during the shrinkage of giant vesicles under electropulsation*, Biophysical Journal **96**, 4109 (2009).

[ACL-235] M. Manghi, J. Palmeri, and N. Destainville, *Coupling between denaturation and chain conformations in DNA: stretching, torsion, bending and finite size effects*, Journal of Physics: Condensed Matter **21**, 034104 (2009).

[ACL-236] N. Destainville, M. Manghi, and J. Palmeri, *Microscopic mechanism for experimentally observed anomalous elasticity of DNA in 2D*, Biophysical Journal, **96**, 4464 (2009).

[ACL-237] N. Ben Amar, H. Saidani, J. Palmeri, and A. Deratani, *Effect of temperature on the rejection of neutral and charged solutes by the Desal 5 DK nanofiltration membrane*, Desalination **246**, 294 (2009).

[ACL-238] N. Ben Amar, N. Kechaou, J. Palmeri, A. Deratani, and A. Sghaier, *Comparison of tertiary treatment by Nanofiltration and Reverse Osmosis for water reuse in Denim textile industry*, Journal of Hazardous Materials, **170**, 111 (2009).

[ACL-239] H. Saidani, N. Ben Amar, J. Palmeri, and A. Deratani, *Interplay between the transport of solutes across nanofiltration membranes and the thermal properties of the thin active layer*, Langmuir, in press (2009).

[ACL-240] J. Palmeri, N. Ben Amar, H. Saidani, and A. Deratani, *Process Modeling of Brackish and Seawater Nanofiltration*, Desalination and Water Treatment, in press (2009).

[ACL-241] C. Sire and S. Redner, *Understanding baseball team standings and streaks*, European Physical Journal B **67**, 473 (2009).

[ACL-242] D. S. Dean, R. R. Horgan, A. Naji, and R. Podgornik, *Thermal Casimir effect between random layered dielectrics*, Physical Review A **79**, 040101 (2009).

[ACL-243] D. Bonamy, P. H. Chavanis, F. Daviaud, B. Dubrulle, and M. Renouf, *Non-linear steady states in dense granular flows*, European Physical Journal B **68**, 619 (2009).

[ACL-244] P. H. Chavanis and L. Delfini, *Dynamical stability of systems with long-range interactions: application of the Nyquist method to the HMF model*, European Physical Journal B **69**, 389 (2009). Highlighted in Europhysics News **40**, 13 (2009).

[ACL-245] D. S. Dean and A. J. Gopinathan, *The non-equilibrium behavior of fluctuation induced forces*, submitted to Journal of Statistical Mechanics, L08001 (2009).

[ACL-246] C. Touya, D. S. Dean, and C. Sire, *Dipole diffusion in a random electrical potential*, Journal of Physics A **42**, 375001 (2009).

2.2 Articles without references (mostly preprints)

[SRP-10] P. H. Chavanis, *Virial theorem for rotating self-gravitating Brownian particles and two-dimensional point vortices*, submitted to Europhysics Letters (2009).

[SRP-11] J.-M. Escoffre, C. Favard, T. Portet, C. Rosazza, E. Phez, D. S. Dean, and M.-P. Rols, *Time scales of electro-mediated membrane permeabilisation and DNA uptake in cells revealed by direct imaging with high temporal resolution*, submitted to Proceedings of the National Academy of Sciences (2009).

[SRP-12] D. S. Dean, R. R. Horgan, A. Naji, and R. Podgornik, *The effects of dielectric disorder on van der Waals interactions in slab geometries*, submitted to Physical Review E (2009).

[SRP-13] A. Naji, D. S. Dean, J. Sarabadani, R. R. Horgan, and R. Podgornik, *Thermal Casimir-van der Waals interaction between randomly charged dielectrics*, submitted to Physical Review Letters (2009).

2.3 Invited talks in international and national conferences

[INV-58] P. H. Chavanis, *Nonlinear mean field Fokker-Planck equations*, invited talk at the *Conference "News, Expectations and Trends in Statistical Physics (NEXT-SigmaPhi)"* (Kolymbari, Creta, 12-19 August 2005).

[INV-59] P. H. Chavanis, *Phase transitions in self-gravitating systems*, invited talk at the *Conference "Statistical Mechanics of Non-Extensive Systems"* (Paris, France, 24-25 October 2005)

[INV-60] D. S. Dean, *Slow dynamics and aging*, invited talk at the *Conference on Slow Dynamics and Aging* (Session on Granular Matter, Institut Henri Poincaré, Paris, France, March 2005).

[INV-61] D. S. Dean, *Thermodynamic approaches to granular media*, invited talk at the *Granular Physics Conference* (KITP, Santa Barbara, USA, June 2005).

[INV-62] D. S. Dean, *A physicist's perspective on optimization problems*, invited talk at the *FCOM Stochastic Computation* (Santander, Spain, June 2005).

[INV-63] D. S. Dean, *The statistics of a slave estimator for response in Langevin systems*, invited talk at the *Recent Progress in Glassy Physics* (Paris, France, September 2005).

[INV-64] D. S. Dean, *Field theoretic methods for transport in random media*, invited talk at the *Conference in honour of Prof. I. T. Drummond* (Cambridge, UK, September 2005).

[INV-65] D. S. Dean, *The statistical mechanics of combinatorial optimization problems with site disorder*, invited talk at the *ECCS'05 Cospico Satellite* (Paris, France, November 2005).

[INV-66] D. S. Dean, *Statistics of a slave estimator*, invited talk at the *Conference on Relaxation Dynamics of Macroscopic Systems* (Isaac Newton Institute, Cambridge, UK, January 2006).

[INV-67] D. S. Dean, *Phase transition in the Aldous Shields Growth Model*, invited talk at the *Conference on First-Passage and Extreme Value Problems in Random Processes* (Isaac Newton Institute, Cambridge, UK, June 2006).

[INV-68] N. Destainville, *Arctic phenomena in random tilings with fixed boundaries*, invited talk at the *DMV-Jahrestagung* (Bonn, Germany, 18-22 September 2006).

[INV-69] A. Ayral, A. Julbe, C. Guizard, J. Sanchez, G. M. Rios, and J. Palmeri, *Use of ceramic nanofilters for the treatment of solvents*, in *Proceedings of the International Workshop on Membranes in Solvent Filtration*, invited talk at the *International Workshop on Membranes in Solvent Filtration* (Leuven, Belgium, 23-24 March 2006).

[INV-70] P. H. Chavanis, *Nonlinear mean field Fokker-Planck equations*, invited talk at the *Conference "Complexity, Metastability and Nonextensivity"* (Catania, Italy, 1-4 July 2007); *AIP Conference Proceedings* **965**, 144 (2007).

[INV-71] P. H. Chavanis, *Systems with long-range interactions: interpretation of the different functionals*, invited talk at the *Conference "Dynamics and Thermodynamics of Systems with Long-range Interactions: Theory and Experiments"* (5-7 July 2007, Assisi, Italy); *AIP Conference Proceedings* **970**, 39 (2008).

[INV-72] N. Destainville, *Flip dynamics and connectivity in 3-dimensional tilings by rhombohedra*, invited talk at the *International Conference on Combinatorics* (Cracow, Poland, July 2007).

[INV-73] A. Deratani, H. Saidani, J. Palmeri, and N. Ben Amar, *Temperature effect on solutes transport in nanofiltration*, invited talk at the *Asian Membrane Society Conference* (Taipei, Taiwan, 16-18 August 200).

[INV-74] D. S. Dean, *Growth models on trees*, invited talk at the *Conference on Interfaces between Physics and Computer Science* (Jacobs University, Bremen, Germany, July 2007).

[INV-75] D. S. Dean, *Extreme value statistics of maximal eigenvalues of random matrices* invited talk at the *III BRUNEL Workshop on Random Matrix Theory* (Brunel, UK, December 2007).

[INV-76] P. H. Chavanis, *Kinetic theory of point vortices in two dimensions*, invited talk at the *IUTAM Symposium "150 Years of Vortex Dynamics"* (Copenhagen, Denmark, 13-16 October 2008).

[INV-77] P. H. Chavanis, *Kinetic theory of point vortices in two dimensions*, invited talk at the *International Conference on Statistical Physics (SigmaPhi2008)* (Kolymbari, Creta, 14-18 July 2008).

[INV-78] D. S. Dean, *Diffusion in non-Gaussian potentials in one dimension*, invited talk at the *Workshop on Statistical Physics and Low Dimensional Systems* (Nancy, France, 21-23 May 2008).

[INV-79] D. S. Dean, *Fluctuation induced interactions in one dimensional Coulomb gases*, invited talk at the *Conference Fluctuate 08* (Santa Barbara, USA, September 2008).

[INV-80] N. Destainville, *Methodological aspects of diffusion analysis by microscopy techniques*, invited talk at the *INSERM Workshop on Physical modeling and mathematical analysis in cellular biology* (St-Raphaël, France, 2008).

[INV-81] N. Destainville, *Mixing times of Markov chains, the multi-decomposition technique, flip dynamics in random tilings*, invited talk at the *Workshop on "Random Tilings, Random Partitions and Stochastic Growth Processes"* (Montréal, Canada, 1-6 September 2008).

[INV-82] N. Destainville, *Apports de la physique théorique à la compréhension de la matière vivante à l'échelle moléculaire*, invited talk at the *Troisième Workshop ITAV* (Toulouse, France, 25 September 2008).

[INV-83] N. Destainville, *Phases "clusters" de protéines membranaires : un nouveau mécanisme de confinement ?*, invited talk at the *GDR Physique de la cellule au tissu* (Sète, France, 2008).

[INV-84] C. Sire, *Poker and statistical physics*, invited talk at the *Conference on Algebraic Statistics, Machine Learning and Lattice Spin Models* (Cold Spring Harbor Laboratory, USA, 16-19 March 2008).

[INV-85] C. Sire, *The out of equilibrium physics of poker tournaments*, invited plenary talk at the *Workshop on Statistical Physics and Low Dimensional Systems* (Nancy, France, 21-23 May 2008).

[INV-86] J. Palmeri, *Brackish and seawater desalination using NF and RO membranes: transport theory, modeling, and process simulation*, invited talk at the *4-day Intensive Course, Middle East Desalination Research Center (MEDRC)* (Casablanca, Morocco, 2-5 February 2009).

[INV-87] J. Palmeri, L. Schrive, and A. Deratani, *Modélisation des procédés de nanofiltration avec le logiciel NanoFlux: applications nucléaires*, invited talk at the *Journées Thématiques "Membranes et Nucléaire" – Club Français des Membranes (CFM)* (Marcoule, France, 15-16 January 2009).

[INV-88] J. Palmeri and M. Metaiche, *Optimization of reverse osmosis and nanofiltration desalination systems*, invited talk at the *Scientific Workshop: Microsoft-CNRS Chair: Optimisation for Sustainable Development - École Polytechnique* (Palaiseau, France, 3 June 2009).

[INV-89] C. Sire, *Dynamics of self-gravitating Brownian particles*, invited talk at the *MGAT9 – Self-Gravitating Systems* session of the 12^{th} *Grossmann Meeting* (UNESCO, Paris, France, 12-18 July 2009).

2.4 Oral communications leading to a conference proceeding

[ACTI-17] S. N. Majumdar, D. S. Dean, and P. L. Krapivsky, *Understanding search trees via statistical physics*, in *Proceedings of the 22nd IUPAP International Conference of Statistical Physics – STATPHYS 22* (Bangalore, India, 4-9 July 2004), *Pramana-Journal of Physics* **64**, 1175 (2005).

[ACTI-18] M. Metaiche and J. Palmeri, *Ion Retention by Nanofiltration: Modelling of Experimental Data by Nanoflux*, in *the Proceedings of the International Forum on Water - Resources, Technologies and Management in the Arab World, Including the 2nd Forum on Water Desalination and Purification Technology Outlook for the Arab World and Non-Governmental Organizations* (Sharjah, United Arab Emirates, 8-10 May 2005), p. 45 (2005).

[ACTI-19] M. Metaiche and J. Palmeri, *Optimisation multi-critères par algorithmes génétiques du design des réseaux d'osmose inverse*, in *Proceedings du Colloque International sur l'optimisation et les systèmes d'information - COSI'07* (Oran, Algeria, 11-13 June 2007), p. 349 (2007).

[ACTI-20] J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Molecular dynamics study of ion partitioning and transport in nanoporous membranes*, in *the Proceedings of Engineering with Membranes 2008* (Algarve, Portugal, 25-28 May 2008), available on CD (2008).

[ACTI-21] J. Palmeri, N. Ben Amar, H. Saidani, and A. Deratani, *Process modeling of brackish and seawater nanofiltration*, in *Proceedings of the MDIW08 Conference (Membranes in Drinking Water Production and Wastewater Treatment)* (Toulouse, France, 20-22 October 2008), paper 277 (available on CD) (2008).

[ACTI-22] M. Metaiche and J. Palmeri, *Development of optimization software of RO systems for water desalination: 'DesaltOp'*, in *the Proceedings of the 3rd International Conference on Water Resources and Arid Environments* (Riyadh, Saudi Arbia, November 2008), p. 31 (2008).

[ACTI-23] M. Metaiche and J. Palmeri, *Optimisation membranaire dans les installations d'osmose inverse sous Desaltop*, in the Proceedings de la 2ème Journée scientifique sur le traitement et la réutilisation des eaux - *JSTRE'08* (Blida, Algeria, 11 March 2008), p. 7 (2008).

[ACTI-24] P. H. Chavanis, G. De Ninno, D. Fanelli, and S. Ruffo, *Out of equilibrium phase transitions in mean-field Hamiltonian dynamics*, in *Proceedings of the Conference on Chaos, Complexity and Transport* (Marseille, France, 5-9 June 2007), p. 3 (2008).

[ACTI-25] P. H. Chavanis, *Generalized Keller-Segel models of chemotaxis. Analogy with nonlinear mean-field Fokker-Planck equations*, in *Proceedings of the Conference on Chaos, Complexity and Transport* (Marseille, France, 5-9 June 2007), p. 256 (2008).

2.5 Oral communications not leading to a conference proceeding

[COM-12] P. H. Chavanis, *Relaxation equations for two-dimensional turbulence*, *Workshop on "Interdisciplinary Aspects of Turbulence"* (Tegernesee, Germany, 18-22 April 2005).

[COM-13] N. Destainville, *Single molecule tracking as a tool to unravel the dynamic membrane organization of the μ opioid receptor*, *CECAM Workshop "Biomembrane Organization and Protein Function – From Computation to Experiment"* (Lyon, France, 4-6 April 2005).

[COM-14] J. Palmeri, N. Ben Amar, H. Saidani, and A. Deratani, *Modeling the membrane nanofiltration (NF) of brackish and sea water*, *EuroMed 2006* (Montpellier, France, 21-25 May 2006).

[COM-15] N. Ben Amar, H. Saidani, J. Palmeri, and A. Deratani, *Temperature dependence of water and neutral solutes transport in nanofiltration membranes*, *Euromembrane 2006* (Taormina, Italy, 24-28 September 2006).

[COM-16] P. H. Chavanis, *Kinetic theory of point vortices in two dimensions*, *Conference "Complex Substances in Turbulence"* (Eilat, Israel, 3-8 November 2007).

[COM-17] N. Destainville, *Phases "cluster" de protéines membranaires : un nouveau mécanisme de confinement ?*, *GDR Microscopie fonctionnelle du vivant* (Marseille, France, 2007).

[COM-18] N. Ben Amar, H. Saidani, A. Deratani, and J. Palmeri, *Temperature effect on rejection of neutral and charged solutes by nanofiltration membrane Desal-5 DK*, *Meda Water International Conference on Sustainable Water Management* (Tunis, Tunisia, 21-24 March 2007).

[COM-19] N. Ben Amar, N. Kechaou, R. Ben Amar, J. Palmeri, and A. Deratani, *Traitements membranaires d'effluents de l'industrie textile et dimensionnement d'une unité de nanofiltration – Cas de la SITEX*, *Technologies de Traitement et de Réutilisation des Eaux Résiduaires Industrielles dans les pays du Bassin Méditerranéen* (Jerba, Tunisia, 24-26 May 2007).

[COM-20] M. Manghi, *Fluctuations govern diffusion in lipid membranes: experimental and theoretical study on controlled stacked membranes*, *GDR Physique de la Cellule au Tissu* (Sète, France, 2008).

[COM-21] N. Kechaou, N. Ben Amar, A. Deratani, and J. Palmeri, *Nanofiltration Tertiary Treatment of a Textile Wastewater in a Denim Facility*, *International Symposium on Biotechnology, ProMembrane International Conference* (Sfax, Tunisia, 4-8 May 2008).

[COM-22] P. H. Chavanis, *Kinetic theory of point vortices in two dimensions*, *Meeting "Turbulence and Statistical Mechanics"* (Les Houches, France, 2-6 March 2009).

2.6 Posters in conferences

[AFF-23] J. Palmeri, X. Lefebvre, P. David, and Z. Twardowski, *L'utilisation du logiciel NanoFlux pour modéliser des procédés de nanofiltration dans l'industrie chimique*, poster presented at the *Conférence CFM (Club Français des Membranes) Applications Industrielles des Procédés Membranaires en Chimie et Production d'Énergie* (Lyon, France, 13-14 June 2005).

[AFF-24] N. Ben Amar, H. Saidani, J. Palmeri, and A. Deratani, *Quels paramètres prendre en compte pour la modélisation de l'effet de la température sur les performances en nanofiltration ? Cas des solutés neutres*, poster presented at the *Conférence MEMPRO 3* (Nancy, France, 5-7 April 2006).

[AFF-25] J. Palmeri, X. Lefebvre, N. Ben Amar, H. Saidani, and A. Deratani, *Brackish and seawater nanofiltration (NF) modeling using NanoFlux software*, poster presented at the *AMTA Biennial Conference, Desalination Comes of Age – The Answer for New Supplies* (Anaheim CA, USA, 30 July-2 August 2006).

[AFF-26] A. Deratani, S. Touil, J. Palmeri, S. Tingry, and S. Bouchtalla, *Pertraction of xylene isomers using cyclodextrin-containing membranes: mass transport mechanism and modeling*, poster presented at the *Euromembrane 2006 Conference* (Taormina, Italy, 24-28 September 2006).

[AFF-27] N. Kechaou, N. Ben Amar, R. Ben Amar, A. Deratani, and J. Palmeri, *Sitex effluent treatment by membrane bioreactor*, poster presented at the *First Maghreb Conference on Desalination and Water Treatment* (Hammamet, Tunisia, 7-10 December 2007).

[AFF-28] C. Mauroy, N. Destainville, C. Lebrun, M. Manghi, E. Haanappel, S. Mazères, and L. Salomé, *Diffusion of lipids in stacked supported bilayers*, poster presented at the *Biophysical Society 52nd Annual Meeting* (Long Beach CA, USA, 2-6 February 2008).

[AFF-29] C. Tardin, P. Rousseau, O. Walisko, N. Destainville, M. Chandler, and L. Salomé, *Insights in the transposition mechanism of the bacterial insertion sequence IS911 revealed by Tethered Particle Motion*, poster presented at the *Biophysical Society 52nd Annual Meeting* (Long Beach CA, 2-6 February 2008).

[AFF-30] J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Ion transport at the water/air and water/nanopore interfaces*, poster presented at the *7th Liquid Matter Conference* (Lund, Sweden, 27 June-1 July 2008).

[AFF-31] N. Kechaou, N. Ben Amar, A. Deratani, J. Palmeri, and A. Sghaier, *Coupling of biological treatment and membrane filtration for the recycling of textile wastewater*, poster presented at the *Fourth International Biennial BioVision Alexandria 2008 Conference* (Alexandria, Egypt, 12-16 April 2008).

2.7 Books or book chapters

[OS-9] H. Chmiel, X. Lefebvre, V. Mavrov, M. Noronha, and J. Palmeri, *Computer Simulation of Nanofiltration, Membranes and Processes*, in *Handbook of Theoretical and Computational Nanotechnology*, Volume 5, edited by Michael Rieth and Wolfram Schommers, pp. 93-214, American Scientific Publishers (2006).

2.8 Vulgarisation publications

[OV-4] N. Destainville, *Systèmes complexes, physique et biologique*, *Magazine scientifique de l'UPS* **4**, 9 (2005).

[OV-5] P. H. Chavanis and C. Sire, *Mettre de l'ordre dans le chaos*, *Magazine scientifique de l'UPS* **4**, 11 (2005).

[OV-6] L. Salomé, P.-F. Lenne, and N. Destainville, *Membranes biologiques : vers un modèle physique*, *Images de la Physique 2006*, p. 74 (CNRS, 2006).

[OV-7] C. Sire, *La physique hors des sentiers battus (Physics off the beaten track)*, popular talk presented on many occasions since 2005 (*Ouvertures de l'UPS*, *Fête de la Science*, high-schools, high-school teachers, students, public conferences... download the *pdf* version in French or English).

[OV-8] C. Sire, *Histoire de la cosmologie moderne : 13.7 milliards d'années en 60 minutes (History of modern cosmology: 13.7 billion years in 60 minutes)*, popular talk presented on many occasions since 2005 (*Fête de la Science*, high-schools, high-school teachers, students, public conferences... download the *pdf* version in French).

[OV-9] C. Sire, *Borel et von Neumann : deux grands mathématiciens précurseurs de la théorie du poker (Borel and von Neumann: two famous mathematicians pioneering the theory of poker)*, article published on the poker blog of the French daily *Libération* (2007); see also the entry reviewing Ref. [ACL-197].

[OV-10] N. Destainville, M. Manghi, and J. Palmeri, *Quand les physiciens se penchent sur l'ADN*, *Magazine scientifique de l'UPS* **11**, 12 (2007).

2.9 Books as Editor

[DO-3] C. Sire, coeditor of *Images de la Physique*, a yearly magazine edited by CNRS exposing recent trends in physics for non specialists (2002-2007).

2.10 Commercial and Open Source softwares

[COD-3] J. Palmeri, P. David, and X. Lefebvre, *NanoFlux*, Commercial software developed by the Laboratoire de Physique Théorique (LPT-UMR 5152, Toulouse) and the Institut Européen des Membranes (IEM-UMR 5635, Montpellier) under the NanoFlux Project. *NanoFlux Software* is an advanced tool for the prediction and scaling-up of nanofiltration membrane processes (research and development and industrial filtration and separation applications). Three licences were recently sold to Université de Nantes, CEA, and Aker Kvaerner Chemetics (Vancouver, Canada).

2.11 Habilitation thesis to supervise researches

[HDR-2] N. Destainville, *Dynamique de flips dans les pavages aléatoires & Dynamique diffusionnelle de récepteurs membranaires (Flip dynamics in random tilings & Diffusional dynamics of membrane receptors)*, Thèse d'habilitation à diriger des recherches, Université Paul Sabatier (29/11/2005).

2.12 PhD thesis completed or in progress

[TH-11] V. Desoutter, *Étude de deux systèmes dynamiques dominés par des phénomènes entropiques (Study of two dynamical systems dominated by entropic phenomena)*, PhD thesis, Université Paul Sabatier (01/10/2001-4/10/2005); supervisor: N. Destainville.

[TH-12] M. Metaiche, *Optimization of reverse osmosis desalination systems, operating parameters and numerical simulations (Optimisation des systèmes de désalination, paramètres opératoires, et simulations numériques)*, PhD thesis (co-direction), École Nationale Polytechnique d'Alger (Algeria) and University de Montpellier II, France (01/10/2004-15/12/2007); supervisors: A. Kettab and J. Palmeri.

[TH-13] J. Sopik, *Dynamique de marcheurs aléatoires en interaction (Dynamics of interacting random walkers*, PhD thesis, Université Paul Sabatier (01/10/2003-26/06/2007); supervisor: C. Sire.

[TH-14] J. Dweik, *Molecular modeling of membrane transport (Modélisation moléculaire du transport membranaire)*, PhD thesis, University de Montpellier II (01/09/2005-19/12/2008); supervisor: J. Palmeri.

[TH-15] L. Horvath, *Molecular dynamics studies of water, ions, and macromolecules in nanopores (Étude de dynamique moléculaire de l'eau, des ions, et des macromolécules dans des nanopores)*, PhD thesis (co-direction), Université Paul Sabatier and University Babes-Bolyai (Cluj-Napoca, Romania) (01/10/2006-$\sim$10/2009); supervisors: J. Palmeri and T. Beu.

[TH-16] C. Touya, *Diffusion dans des potentiels aléatoires non gaussiens (Diffusion in non-Gaussian random potentials)*, PhD thesis, Université Paul Sabatier (01/10/2006-$\sim$30/09/2009); supervisor: D. S Dean.

[TH-17] T. Portet, *Étude de l'électroperméablisation de vésicules artificiels (Study of the electropermeabilisation of artificial vesicles)*, PhD thesis, Université Paul Sabatier (01/10/2007-$\sim$10/2010); supervisors: D. S Dean and M.-P. Rols (IPBS).

[TH-18] V. Demery, *Modèles physiques pour l'électroperméabilisation des membranes (Physical models of membrane electropermeabilization)*, PhD thesis, Université Paul Sabatier (01/10/2009-$\sim$30/09/2012); supervisor: D. S Dean.