## Terms from theoretical physics of relevance for complex systems science

## Annick LESNE

Laboratoire de Physique Théorique de la Matière Condensée, Case Courrier 121, Université
Pierre et Marie Curie, 4 place Jussieu, 75252 Paris cedex 05, France
lesne@lptmc.jussieu.fr

**Additivity:** a quantity A is additive if its overall value in a system S is the sum of its partial values in the sub-systems composing S, whatever the partition is:  $A(S) = \sum_i A(S_i)$  where  $S = \bigcup_i S_i$ . On the mathematical standpoint, an additive function satisfies f(x+y) = f(x) + f(y) for any pair (x,y); provided it is continuous, it reduces to a linear function f(x) = ax, supporting the following interpretation of additivity: knowing a sample is enough to grasp the collective behavior, thus justifying reductionist approaches and linear\* reconstruction.

**Asymptotic:** refers to the behavior or properties observed in the limit  $t \to \infty$  of the system evolution\*.

Attractor: closed invariant indecomposable subset of the phase space\*, which attracts all trajectories starting sufficiently nearby (in a neighborhood called its basin of attraction), hence fully accounting for the asymptotic\* properties of the dynamical system\*. An attractor is termed a strange attractor if the dynamics restricted on it is chaotic\*.

Average: this term associated with mean values of observable quantities is actually ill-defined; it is essential to precise whether it refers to a *time average* along the system trajectory in the phase space\*, a *spatial average* in case of a spatially extended system observed at different resolutions, or a phase-space average. In this latter case, it is termed a *statistical average* and it involves some weight (a "measure") over the phase space. Ergodic\* theory gives conditions under which time and statistical averages can be identified. For a sample of N independent and identically distributed random variables  $(X_i)_i$ , the *law of large numbers* states the convergence as  $N \to \infty$  of the sample average  $(1/N) \sum_{i=1}^N X_i$  to the common statistical average  $\langle X \rangle$ .

**Bifurcation:** any qualitative change in the asymptotic\* behavior of a dynamical system\* (e.g. an exchange of stability between two fixed points, or the appearance of a limit cycle\*) as a control parameter\* is varied. The parameter value at which the change occurs is the *bifurcation point*. The *bifurcation diagram* is the plot of the attractor(s)\* vs the control parameter. A bifurcation is said to be generic\* if the conditions for observing it are structurally stable\*, i.e. are robust\* with respect to a sufficiently small perturbation\* of the evolution law. The effect of a perturbation would only be to shift the bifurcation point.

**Boltzmann distribution:** relative weight of the different states x of a system; more precisely, it is a probability distribution in the system configuration space, reflecting quantitatively the balance between thermal energy  $k_BT$  (where T is the temperature\* and  $k_B$  the Boltzmann constant) and

potential energy U energies:

$$P_T(X) = \frac{1}{\mathcal{Z}(T)} e^{-U(X)/k_B T}$$

The normalization factor  $\mathcal{Z}(T)$  is called the *partition function* and it gives access through differentiation to several thermodynamic quantities.

Boundary conditions: prescribing the values or behavior of observable quantities at the spatial boundaries of the system is essential to get a well-posed problem.

*Periodic boundary conditions*, i.e. replacing a *n*-hypercube by a *n*-torus by identifying and gluing together the opposite sides, is a numerical trick to simulate an infinite system and avoid issues related to boundaries, e.g. surface effects (but finite-size effects remain).

Catastrophe: a bifurcation\* in the special case of a gradient\* dynamics  $dx/dt = -\nabla U(x, \vec{a})$  depending on some control parameters\*  $\vec{a}$ . The attractors\* are then fixed points  $x_{eq}(\vec{a})$  that might disappear, loose or exchange stability\* as  $\vec{a}$  vary. The topological structure of the surface  $[\vec{a}, x_{eq}\vec{a})]$  and the nature of the singularity\* at the bifurcation point have been classified by René Thom in 7 types, now termed "elementary catastrophes".

Cellular automata: dynamic model where the time, the space and the states take only discrete values, specified by the time step  $\Delta t$   $(t_n = n\Delta t)$ , the spatial lattice, e.g. a square lattice of parameter a  $(x_i = ia, y_j = ja)$  and a countable or more often finite set of elementary states (state of the cell (i, j) at time n). Such a model is specially well suited for numerical simulations. It allows to determine the wealth of possible collective dynamic behaviors achieved with a minimal set of dynamic rules, hence to evidence generic\* mechanisms that might explain self-organization\* and various other emergent\* properties (for instance spontaneous segregation and pattern formation, traveling waves, synchronization). A cellular automata is said to be deterministic\* if the updating rules (specifying the state at time n+1 knowing the state at time n) are deterministic, or stochastic\* if they involve random\* choices.

Chaos: a peculiar regime observed in some deterministic,\* low-dimensional dynamical systems\*, characterized by an erratic, impredictible behavior at long times while the short-term behavior is perfectly predictible. Three ingredients are required to get a chaotic regime: sensitivity to initial conditions, reflecting in the existence of at least one strictly positive Lyapounov exponent\*, mixing (in particular, the dynamics should remain in a bounded region), and the existence of a dense infinity of unstable periodic orbits. A continuous-time dynamics requires a phase space\* of dimension at least 3 to exhibit chaos. On the technical side, two standpoints, either topological or measure-theoretic, can be adopted to describe and measure chaotic features.

A scenario toward chaos is a well-defined sequence of bifurcations\* leading from an equilibrium situation (a dynamical system with a stable fixed point) to a chaotic one.

Characteristic time: typical time scale of a phenomenon. Quantitatively, it is the period in case of an oscillatory behavior, the relaxation time  $\tau_r$  in case of an exponential decay  $e^{-t/\tau_r}$ , or more generally the time over which some relevant observable A varies:  $\tau_A = \langle |A(t)/A'(t)| \rangle$  where  $\langle \rangle$  indicates some local time average.

Closure: when restricting the description of a large system to that of a sub-system, one usually needs to add extra relations (more often approximate) called *closure relations*, to get closed equa-

tions involving only the variables relative to the considered sub-system.

Coarse-graining: multi-scale procedure allowing to reduce the complexity of a given model by performing local averages to get a coarser (i.e. with a lower resolution) description of the system. It can be implemented either in real space (for a spatially extended system), either in phase space\*. Typically, one introduces a partition in cells and performs a space (respectively a phase-space) average over each cell in order to reduce its description to that of a few degrees of freedom. In general some approximations (closure\* relations) are required to get closed equations for these coarser, effective\* degrees of freedom.

**Complexity:** beyond the current meaning of this name, one encounters several notions of complexity in theoretical physics. Let us cite among others the algorithmic complexity of a symbolic sequence, actually an entropy\*. A true notion of complexity has been defined in dynamical systems\* theory, as the speed of convergence of the finite-time entropy rates  $H_n/n$  towards their limit h (the Kolmogorov-Sinai entropy\*):

$$c = \sum_{n=1}^{\infty} (H_n - nh) = \sum_{n=1}^{\infty} (2H_n - H_{2n})$$

In the case of the logistic map family  $[f_a(x) = ax(1-x)]_{1 \le a \le 4}$ , one has c(4) = 0 whereas the entropy is there maximal:  $h(4) = \log 2$  (a fully chaotic behavior is observed for a = 4); on the contrary, one has  $h(a_c) = 0$  at the chaotic threshold  $a_c$  whereas  $c(a_c) = \infty$ .

**Conditional probability:** probability P(A|B) of an event A knowing that an event B has occurred. According to the Bayes rule, P(A|B) = P(A,B)/P(B) hence P(A|B) = P(B|A)P(A)/P(B).

Conformation: 3-dimensional shape of a macromolecule, taken as its microscopic state in statistical mechanics studies of conformational transitions, folding or allosteric transitions.

Conjugate space: defined by contrast to the *real space*, in which the observable quantities  $\mathcal{A}$  are described as spatio-temporal fields  $A(\vec{r},t)$ . "Working in conjugate space" means to represent these observables as functions  $\widehat{A}(\vec{q},\omega)$  of the frequency  $\omega$  and wave vector  $\vec{q}$ . The correspondence between real space and conjugate space is usually achieved by Fourier or Laplace transformations, allowing to perform explicitly the decomposition of sufficiently well-behaved fields  $A(\vec{r},t)$  (e.g. square-integrable) into components  $\widehat{A}(\vec{q},\omega)$ :

$$\widehat{A}(\vec{q},\omega) = \int e^{i\vec{q}.\vec{r}} \; A(\vec{r},t) \; \frac{d^3\vec{r} \; dt}{4\pi^2}, \quad \text{and conversely} \quad A(\vec{r},t) = \int e^{i\vec{q}.\vec{r}} \; \widehat{A}(\vec{q},\omega) \; \frac{d^3\vec{q} \; d\omega}{4\pi^2}$$

The conjugate representation straightforwardly gives the contribution  $\widehat{A}(\vec{q},\omega)$  at time scale  $2\pi/\omega$  and spatial scale  $2\pi/q$  to the observable  $\mathcal{A}$ . Small spatial scales correspond to large wave vectors  $q \to \infty$  and similarly for the time scales. One speaks of *ultraviolet (UV) behavior* (for instance an UV divergence\*) if it occurs for  $q, \omega \to \infty$  and *infrared (IR) behavior* (e.g. an IR divergence) if it occurs for  $q, \omega \to 0$ , in reference to the corresponding ordering of colors and frequencies in light.

**Conservation:** the existence of invariants, i.e. conserved quantities, in the course of the evolution\* of a given system, reflects in conservation equations, e.g. the *continuity equation*  $\partial n/\partial t + \vec{\nabla} \cdot \vec{\jmath} = 0$ , where  $n(\vec{r},t)$  is the local density and  $\vec{\jmath}(\vec{r},t)$  the local density of current. The right-hand-side can be

supplemented with a source term, if any. Similar equations can be written for different pairs  $(n, \vec{j})$ , for instance the (density, density of current) of charge, energy or impulsion in an isolated system.

Conservative: refers to a dynamical system\* in which the total energy is conserved (by contrast to a dissipative\* one). Its evolution is described by Hamilton equations and the natural volume of the phase space is conserved by the dynamics (Liouville theorem).

Continuous medium: approximation replacing the molecular description of a many-particle system by that of a continuous field of matter; it is valid at large enough scale, such that the elementary volume  $d^3\vec{r}$  contains an enough large number  $N\gg 1$  of particles to neglect their discrete nature and ensuing discontinuous variations, and to get a *continuous* density field. This number N is also supposed to be enough large to neglect fluctuations inside a cell  $d^3\vec{r}$ , so as to adopt a deterministic\* description, identifying the actual density with its statistical average.

Control parameter: any tunable parameter whose value controls the relevant behavior of the considered system, e.g. the temperature or coupling strength when investigating a phase transition\*, the strength of nonlinearitites when studying the bifurcations\* of a dynamical system, the ionic strength when studying the conformational\* transition of a charged macromolecule.

**Coupling:** direct interaction between two elements. It is usually described by an interaction potential  $V(x_1, x_2)$  depending on the states  $x_1$  and  $x_2$  of the two elements (including their positions  $\vec{r}_1$  and  $\vec{r}_2$  in real space). The *coupling strength* is the typical energy involved in the interaction, whereas the *coupling range* is the distance  $|\vec{r}_1 - \vec{r}_2|$  up to which the elements actually experience their mutual influence.

Coupling should not be confused with correlation\*, that is a statistical relationship between the two elements (it might exist even in the absence of any coupling, as for instance in percolation\* lattices). Nevertheless, it is often the case in multi-scale modeling that correlations at a given level of description are accounted for as an effective\* coupling in a coarse-grained\* description.

**Correlation:** statistical dependence between two sub-systems or more generally, two random variables A and B. In case of a process A(t) or a spatially extended variable  $B(\vec{r})$ , one defines (auto)-correlation functions as follows:

$$C_A(t) = \langle A(t)A(0) \rangle - \langle A(t) \rangle \langle A(0) \rangle \qquad C_B(\vec{r}) = \langle B(\vec{r})B(\vec{0}) \rangle - \langle B(\vec{r}) \rangle \langle B(\vec{0}) \rangle$$

where  $\langle \ \rangle$  denotes the statistical average. In practice, such correlation functions are computed as time or space average, using an argument of ergodicity\*, e.g.

$$C_A(t) \approx \frac{1}{T-t} \sum_{s=0}^{T-t-1} A(t+s)A(s) - \left(\frac{1}{T-t} \sum_{s=0}^{T-t-1} A(t+s)\right) \left(\frac{1}{T-t} \sum_{s=0}^{T-t-1} A(s)\right)$$

The normal behavior of correlations is to be exponentially decaying, thus defining a correlation time  $\tau_c$  (such that  $C_A(t) \sim C_A(0) e^{-t/\tau_c}$ ) and a correlation length  $\xi_c$  (such that  $C_B(\vec{r}) \sim C_B(\vec{0}) e^{-r/\xi_c}$ ). A slower decay, e.g. as a power law\*, reflects a divergence of the correlation time/length, or equivalently a critical\* character of the system.

Critical: critical points in physics have had for many years a clearly delineated meaning, in thermodynamics: an isolated point where a phase transition\* of a special kind ("second-order phase

transition") occurs. In the phase diagram\* of the system, in coordinates [pressure, temperature], it is a point ending a line of coexistence between two phases, say liquid and vapor. The system there exhibits special features: almost macroscopic inhomogeneities in its density, divergence of susceptibility and other response functions, singularity in its free energy\*. Since the 70's and the development of renormalization\* methods, critical phenomena have been recognized in many other fields: percolation\*, conformation of a polymer chain, growth, turbulence. The main signature of a critical point is the presence of long-range correlations, reflecting in the divergence of correlation\* length and time and power-law\* behavior of the correlation functions (instead of an exponential decay). Accordingly, it is associated with large fluctuations, anomalous response properties to perturbations and scaling\* laws for the order parameters\* and susceptibilities. The meaningful quantities to quantitatively describe a critical behavior are thus the *critical exponents* involved in these power laws.

A specific instance is self-organized criticality\*, in which the system spontaneously reach a critical point (i.e. with no need to tune from outside one of its control parameter\*).

By contrast, it is to note that in mathematics, a critical point of a function f(x) is simply an extremal point  $x_c$  (such that the derivative  $f'(x_c) = 0$ ) and where f takes a (locally) extremal value. Considering a dynamical system dx/dt = F(x), a critical point is an stationary point  $x_c$  such that  $F(x_c) = 0$ ; it corresponds to a critical point of the potential U(x) in case of a gradient dynamics F = -dU/dx.

**Detailed balance:** relation satisfied at equilibrium in any system evolving according to a Markov process, i.e. whose evolution is fully determined by the transition probabilities between two successive times with no further memory\*. Considering for simplicity the case of discrete time and discrete states, the detailed-balance relation writes  $W_{ij}p_j(\infty) = W_{ji}p_i(\infty)$  for any pair (i,j) of states, where  $W_{ij}$  is the transition probability from j to i (i.e. the conditional probability\* of observing the state i at time t+1 knowing that the state is j at time t) and  $p(\infty)$  the stationary distribution, such that  $Wp(\infty) = p(\infty)$ . This relation fails to be satisfied in non equilibrium\* situations, where non vanishing probability currents  $J_{ij} \equiv W_{ij}p_j(\infty) - W_{ji}p_i(\infty) \neq 0$  are still present in the asymptotic, stationary state  $p(\infty)$ .

A formally similar relation is encountered in the context of *chemical kinetics*, expressing that a given reaction is separatedly at equilibrium, notwithstanding the other reactions in which the different species might be involved. It also fails in non equilibrium situations, where fluxes of matter cross the system, even once a stationary state is reached, if any.

**Deterministic:** far from any philosophical idea of determinism or determination, this adjective simply refers to a class of equations used to model the system evolution\*, namely ODE\* or PDE\*, or more generally a set of updating rules such that the knowledge of the system state at time t thoroughly determines its future state. It is to be opposed to stochastic\* models, in which random\* choices are involved in the updating.

**Diffusion:** a mode of transport of particles (from molecules up to micron-size grains) in a solvent originating in the elastic collisions of solvent molecules onto the particles. The resulting irreversible\* motion observed at macroscopic scales is thus a statistical consequence arising from a microscopic random motion. The same phenomenon is described at macroscopic scale by a PDE\* (the diffusion equation) for the particle density  $\partial n/\partial t = D\Delta n$ , where D is the diffusion coefficient, and at the mesoscopic\* scale of the particles by a random walk\*. The mean-square displacement  $R^2(t) \equiv$ 

 $\langle |\vec{r}(t)-\vec{r}(0)|^2 \rangle$  of a particle obeys the normal diffusion law  $R^2(t) \sim Dt$  with the same coefficient D. A fully deterministic\* description can also be considered at microscopic scale, accounting for the collisions of the solvent molecules and the particles. This example underlines that the deterministic or stochastic\* nature of a dynamics is highly dependent of the scales and phase space in which it is considered: it is essentially a feature of the mathematical model and not an intrinsic property of the actual phenomenon.

**Dimension:** this term is to be understood according to the context, since it might refer to the linear size of the system, to the real space (the line if d=1, the plan if d=2, the usual space if d=3, or abstract spaces if  $d\geq 4$ ) underlying the system, to the number of independent degrees of freedom (dimension of the phase space) and finally, to the unit of a given observable (e.g.  $k_BT$ , where T is a temperature\*, has the dimension of an energy and the ratio  $U/k_BT$ , where U is a potential, energy is said to be dimensionless).

**Dissipative:** in which matter or energy is "consumed", i.e. brought up in the external medium, generally as heat. If not fed, a dissipative system relaxes\* toward equilibrium\* (e.g. a pendulum with friction). If fed continuously, it might reach a non trivial steady state\*, differing from equilibrium insofar as fluxes cross the system and the entropy\* production is strictly positive.

**Distribution:** the most current meaning is encountered in the probabilistic framework where a distribution function describes the law of probability of a random\* variable. A related but restricted meaning is that of *generalized function* introduced by Schwartz, e.g. the Dirac distribution  $\delta$ .

**Divergence:** this ambiguous term first designates a linear differential operator transforming a vector field\*  $\vec{v}(\vec{r},t)$  into a scalar field  $\vec{\nabla}.\vec{v}(\vec{r},t)$  (in Cartesian coordinates  $\vec{\nabla}.\vec{v} = \sum_i \partial v_i/\partial x_i$ ). It is also associated with various singularities\* where infinite quantities appear, for instance the divergence of the correlation length at a critical\* point.

**Dynamic:** evolving in the course of time; it thus differs from the biological meaning of "exhibiting an alternation of assembly and disassembly events".

**Dynamical system:** a mathematical model of the form dX/dt = V(X,t) describing the evolution\* of a system whose instantaneous state is represented by some point X of a vector space of a manifold (the *phase space* of the system). It is to note that such a model is memoryless\*, without delay and deterministic\* insofar as the knowledge of the system state X(t) at the single time t thoroughly determines its future evolution. The dynamical system is said to be *autonomous* if V does not explicitly depend on t.

Effective parameter: parameter of a mesoscopic\* model accounting in an integrated way of far more complex phenomena occurring at lower scales. For instance, an effective diffusion\* coefficient might be introduced to summarize the average effect of small-scale obstacles thus avoiding to describe them explicitly; an effective coupling\* constant might reflect the net effect of direct and also indirect interactions taking place at a lower scale; an effective stochastic\* process is generally required in the coarse-grained\* description of a deterministic\* flow, since many trajectories now originate from the same "mesoscopic point".

**Element:** any kind of sub-system chosen to be described as a structureless entity.

Emergence: refers to any collective property or behavior that cannot be predicted from the properties and behavior of a single element, but involves essentially the interactions between the elements. Acknowledged physical examples of emergence are irreversibility \* and phase transitions\*. One might suggest that a specific feature of complex systems is the feedback of emerging properties onto the very features and potentialities of the elements, thus allowing the observation of non generic\* situations, e.g. marginally stable or even critical\* situations, through inter-level coupling.

**Entropy:** this term unfortunately recovers a host of different notions, somehow related, but that should be carefully distinguished. Here follows a brief definition of the main ones.

Historically the first notion is the thermodynamic entropy: in thermodynamics\*, one assumes the existence of a state function  $S_{th}(U,V,N)$  depending on the volume V, the particle number N (or  $N_1,\ldots,N_q$ ) in case of a q-component system) and internal energy U; its derivatives yield thermodynamic quantities, e.g. the temperature through  $(\partial S_{th}/\partial U)_{V,N}=1/T$ . The free energy\* is defined as  $F=U-TS_{th}$ .

A statistical notion has later been introduced by Boltzmann for isolated systems: the *Boltzmann* entropy of the system is  $S_B = k_B \log \Omega$  where  $\Omega$  is the number of possible states of the system. Assuming that states are equally accessible, this entropy coincide with the thermodynamic one.

This notion have been extended by Gibbs at a slightly higher scale ("mesoscopic" scale), at which the state of the system is described by a continuous variable x; denoting by  $\rho(x)$  its distribution function, the *statistical* (Gibbs) entropy of the system is  $S_G = -k_B \int \rho(x) \log \rho(x) dx$ . At thermal equilibrium,  $\rho(x)$  is the Boltzmann distribution\* and here again,  $S_G$  coincide with the thermodynamic entropy, up to an additive constant related to the coarse-graining\* involved in the definition of the mesoscopic state x and continuous distribution  $\rho(x)$ .

In a totally different context, that of communication theory (now acknowledged as "information" theory"), Shannon introduced a formally similar notion of entropy, also called *information*: considering an event with discrete outcomes i = 1 ... n, with probability  $p_i$ , the information gained in observing the outcome i (or equivalently the missing information before observing the outcome, the greater as the outcome is a "surprise") is defined to be  $\log(1/p_i)$ , yielding the expression  $I = -\sum_i p_i \log p_i$  for the average information.

Entropy has been extended to dynamic processes into a notion of entropy rate h (Kolmogorov-Sinai entropy) measuring the information generated at each time step:  $h = \lim_{n\to\infty} H_n/n$  where  $H_n = I[p^{(n)}]$  and  $p^{(n)}$  describes the possible n-step trajectories (more precisely, one has moreover to introduce a partition of the phase space to get discrete trajectories, then let the size of the partition cells tends to 0). A strictly positive entropy h > 0 is a hallmark of chaotic\* behavior.

Finally, on still different grounds, Kolmogorov introduced the notion of algorithmic complexity of a symbolic\* sequence, namely the length of the shorter program that might generate this sequence. For an ergodic symbolic evolution, it can be shown that almost all trajectories have the same algorithmic complexity, coinciding with the above-mentionned entropy rate h.

Entropic effect: apparent force resulting from the statistical trend towards macroscopic states of larger entropy (typically encountered in macromolecular conformations or colloidal mixtures).

**Equilibrium:** given a time scale and a level of description, i.e. a set of quantities thoroughly describing the system state at this level, the system is said to be "in equilibrium" if these quantitites do not vary in time over the considered time scale; they might vary on a larger scale; they might be the overall consequence of many fluctuating or evolving processes at lower scales. As summarized

by Feynman, "equilibrium occurs when fast variables have relaxed and slow ones not yet begun to evolve".

**Equipartition:** at thermal equilibrium, any degree of freedom is endowed with the same energy  $k_BT/2$  (the characteristic thermal energy) where T is the temperature\* and  $k_B$  the Boltzmann constant.

**Ergodicity:** the operational definition of ergodicity is the *ergodic property*, namely the equality of time and statistical averages\*. It thus involves some weight (a "measure")  $\mu$  in the phase space\*, coinciding with the frequency of visit in phase space regions A:

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T \mathbf{1}_A(x_t) dt = \int \mathbf{1}_A(z) d\mu(z) \qquad \text{or} \qquad \lim_{T \to \infty} \frac{1}{T} \int_0^T \Phi(x_t) dt = \int \Phi(z) d\mu(z)$$

for any integrable function  $\Phi$ . The Birkhoff ergodic theorem gives conditions, in a measure-theoretic framework (the "ergodic theory") under which a given deterministic\* dynamics satisfies the ergodic property: a flow  $(\varphi_t)_t$  in the phase space  $\mathcal X$  satisfies the ergodic property with respect to a measure  $\mu$  if it leaves  $\mu$  invariant and if any invariant subset (namely A such that  $\varphi_t(A) = A$  for any t) is of zero or full measure (i.e.  $\mu(A) = 0$  or  $\mu(\mathcal X - A) = 0$ ); or equivalently if any invariant function F (namely  $F \circ \varphi_t = F$  for any t) is  $\mu$ -everywhere constant. This notion of ergodicity can be extended to Markov\* chains, where it simply requires that any two states of the system can be related by some path in a finite time.

The ergodic hypothesis introduced by Boltzmann in the foundation of statistical mechanics assumes that the microscopic dynamics of an isolated many-particle system is ergodic with respect to the microcanonical distribution, giving the same weight to any state of the energy surface on which the system is confined. Although intuitively supported by molecular chaos (i.e. the chaotic\* nature of molecular dynamics), it is rarely proven and in fact, it is presumably false in most real cases, but with so slight violations that all happens as if it were satisfied, in particular for computational purposes.

**Estimation:** beyond the current meaning of approximate evaluation of a given quantity, this term and its more specific companion "estimator" refer to relations expressing statistical averages, or more generally parameters of a model, from the knowledge of a sample or a time series. The estimator is thus a random\* variable, converging to the desired value (unbiased estimator) or a related value (biased estimator) as the sample size tends to infinity (see for instance the example of correlation functions\*).

**Evolution:** in physics, change of the system state in the course of time. In mathematics, the equation or set of equations (either deterministic\* or stochastic\*, and either discrete or continuous in time, space or phase space\*) describing such a change. It thus strongly differs from the biological meaning encountered in the context of Darwinian theory, where it refers to the observable consequences of natural selection at species level (possibly extended to virus, cells, immune systems, or even molecular species).

Extensivity: a key property of macroscopic systems (in particular required in the framework of thermodynamics\*) according which basic observable quantities (volume, energy, entropy), known as "extensive variables", scale as the total number N of particles of the system. It amounts to a joint property of additivity\* (say, the energy of the system is the sum of the energies of its

sub-systems, whatever the partition is) and homogeneity\* (say, the energy of two sub-systems of identical composition are equal). Accordingly, by dividing the above quantities by N, one obtains intensive variables (energy density, entropy density, specific volume) taking the same value in any sub-system, on a par with other intensive variables as the temperature, the pression or the chemical potential controlling the thermodynamic equilibrium state of the system. Extensivity implicitely encloses a condition of local thermodynamic equilibrium (Dobrushin-Lanford-Ruelle conditions) and requires that only short-range couplings\* are present in the system, so as to neglect surface energies and interfacial energies between the sub-systems. It allows to consider the thermodynamic limit  $N \to \infty$ , N/V = cte and to ignore finite-size\* fluctuations\* and specific influence of the boundaries (e.g. surface effects).

**Field:** a smooth spatio-temporal function representing a spatially extended and time-varying feature of a system considered as a continuous medium\*. Let us cite some representative examples: the temperature field in a piece of metal, the velocity field in a moving fluid, the electromagnetic field. According to its number of components and the (constrained) way it is transformed upon a change of reference frame, the field is a scalar, a vector, or a tensor field.

Finite-size effects: any discrepancy between the actually observed behavior and the behavior expected in the limit as  $N \to \infty$  (where N is the number of particles in the system) or  $L \to \infty$  (where L is the linear size of the system). In the context of phase transitions\*, a finite size  $N < \infty$  smoothes out the singularity\* characterizing the transition: strictly, there is no longer a phase transition in a finite-size system. It is to be underlined that the limits  $N \to \infty$  and  $T \to T_*$  (where  $T_*$  is the temperature of the phase transition) do not commute, in agreement with the singular behavior observed for  $N = \infty$  as  $T \to T_*$  while the behavior is regular in  $T = T_*$  for any finite N.

In the context of critical\* phenomena, a finite size  $L<\infty$  induces a cutoff of the critical divergences\*: the correlation length  $\xi$  no longer diverges, since it is obviously bounded by L. Scaling\* are then only approximately satisfied, unless one explicitly accounts for the L-dependence: this yields extended scaling relations, involving an extra scaling variable  $\xi/L$  but the same critical exponents, known as finite-size scaling relations. Now the very study of the finite-size effects would give access to the (infinite-size) critical exponents.

At molecular scales, a finite value of N is associated with statistical fluctuations\*: the discrepancy with respect to the limiting law of large numbers (stating the equality between the sample and statistical averages in the limit as  $N \to \infty$ ) reflects in the still stochastic nature of all the system properties, e.g. its density, its energy, or the fluxes in and out in case of diffusing or reacting species.

Fluctuations: random, uncontrolled variations of the system state. More specifically, this notion presupposes that some level of description has been chosen, in which part of the system composition or evolution appears as a random phenomenon, typically due to the coupling of the observed quantities with others degrees of freedom (external or at smaller scales) ignored at this level of description. For instance, the number of molecules present in a given region of a gas fluctuates, whereas it can be followed exactly at the level of molecular dynamics: here appears a subjective difference between variations and fluctuations according to the considered setting. An ubiquitous instance of fluctuating behavior is associated with thermal fluctuations, originating in the kinetic energy  $k_BT$  (where T is the absolute temperature\* and  $k_B$  the Boltzmann constant) stored in any degree of freedom at thermal equilibrium.

Fluctuation-dissipation theorem: it states the equality of correlation functions\* (variance of internal fluctuations\*) at thermal equilibrium and response functions (describing the linear\* response of the system to a small excitation). Namely, a system at thermal equilibrium reacts in the same way to external perturbations (a small applied field) and internal ones (fluctuations), and the knowledge of its equilibrium statistics gives a full access to its dynamics in the linear regime. This theorem fails in non equilibrium\* systems (either in metastable\* states or in steady states far from equilibrium).

Fokker-Planck equation: PDE\* describing the evolution of the distribution function P(X,t) of a diffusion process (a Markov\* process with no jumps) equivalent to a Langevin\* equation for X(t). The simplest example is provided by the Fokker-Planck equation  $\partial P/\partial t = D\vec{\nabla}.(P\vec{\nabla}U/k_BT + \vec{\nabla}P)$  describing Brownian motion in a potential energy landscape U(X) at thermal equilibrium.

Fractal: self-similar structure (i.e. such that any magnified detail is similar to the whole pattern) that escapes the Euclidean geometry in the following way: the "mass" M(R) contained in a region of radius R satisfies the scaling law:  $M(kR) = k^{d_f}M(R)$  where  $d_f$  differs from the dimension d of the space and takes in general a non integer value. If a is the resolution (minimal scale of observation), self-similarity writes  $M(ka,kR) = k^dM(a,R)$  or equivalently, introducing the number N(a,R) of cells of linear size a required to cover a region of linear size R of the structure: N(ka,kR) = N(a,R). It follows that  $N(ka,R) = k^{-d_f}N(a,R)$  and  $M(ka,R) = k^{d-d_f}M(a,R)$ . In consequence, the mass (length for a curve, area for a surface) of a fractal structure is ill-defined since it depends on the resolution. The relevant quantitative characteristic feature is now provided by the exponent  $d_f$ , called the fractal dimension. Self-similarity has to be checked before computing the fractal dimension, otherwise  $d_f$  might depend on the scale hence loose any relevant meaning. Only mathematical structures are strictly fractal; in the real world, a fractal structure exhibits the above scaling behavior only in a statistical sense, and in a limited window  $[R_{min}, R_{max}]$  of scales, below and above which an Euclidean behavior is recovered.

Free energy: thermodynamic potential to be minimized at equilibrium at a fixed temperature. It expresses as F = U - TS in thermodynamics\* (U being the internal energy, T the temperature and S the thermodynamic entropy) or as  $F = -k_B T \log Z$  where Z is the partition function in statistical mechanics\*, at the level of microscopic or mesoscopic\* configurations of the system. Its expression reflects the balance between order induced by interactions and disorder due to thermal motion, at work in any classical physical system and at the origin of thermal phase transitions\*.

**Function:** far from the biological notion related to the achievement of some goal or adapted mechanism essential to the preservation of life and reproduction, a function in physics is merely any relationship between a given quantity and other ones taken as variables; for instance the pressure is a function of volume and temperature in equilibrium thermodynamics. With some tolerance with respect to the mathematical notion of function, the same quantity can be considered as a function of different sets of variables.

Functional: any relationship in which the "variable" is not a point or a vector but a function  $f \in \mathcal{F}$ . A delicate point in manipulating functionals is to properly prescribe the functional space  $\mathcal{F}$  and its topological structure.

Gaussian: a class of random variables and stochastic processes, distributed according to Gaussian

statistics

$$P_{m,\sigma}(x) = \frac{1}{\sqrt{2\pi} \sigma} e^{-(x-m)^2/2\sigma^2}$$

A Gaussian random variable is thus fully determined by its first two moments (mean  $\langle X \rangle = m$  and variance  $\langle X^2 \rangle - m^2 = \sigma^2$ ). Any higher-order moment\*  $\langle X^n \rangle$ ,  $n \geq 3$ , can be expressed as a function  $M_n(m, \sigma)$ . The sum of independent Gaussian variables is still Gaussian.

**Gradient:** linear differential operator associating to a smooth scalar field  $A(\vec{r})$  a vector field  $\vec{\nabla}A(\vec{r})$  locally pointing in the direction of steepest descent, or equivalently orthogonal to the level surfaces  $A(\vec{r}) = cte$ . In Cartesian coordinates  $\vec{r} = (x, y, z)$ , its components are  $(\partial A/\partial x, \partial A/\partial y, \partial A/\partial z)$ ; its invariant definition is  $dA = \vec{\nabla}A(\vec{r}).d\vec{r}$ , from which follows its expression in any system of coordinates. The gradient of a potential energy defines a force field.

The *gradient method* is the numerical implementation of an intuitive idea for finding the minimum of an energy landscape, namely following its gradient, i.e. a steepest-descent path.

A gradient dynamics is a dynamical system\*  $d\vec{r}/dt = -\vec{\nabla}V(\vec{r})$  ruled by the gradient of a potential  $V(\vec{r})$ ; accordingly, the equilibrium points (fixed points) coincide with the extrema of V, the stable ones corresponding to the minima of V.

Genericity: a generic condition is a condition that is not affected by a small change in the setting; for instance, imposing the bounds 300 < T < 400 on the temperature is a generic condition whereas the condition T = 100 is not. A "generic property" is obtained under generic conditions. A "generic object" exhibits generic properties: one e.g. speaks of a generic bifurcation\*. It is related to the notions of robustness\*, universality\* and structural stability\*. A quasi synonym is typical. In a probabilistic framework, generic means with probability 1, or in a weaker sense, with a finite (i.e. non vanishing) probability.

**Homogeneity:** statistical invariance\* under spatial translations. In consequence, samples of identical sizes have the same statistical properties whatever their localizations in the system.

**Hydrodynamic:** beyond the reference to fluid dynamics theory, hydrodynamic description is a shorthand to designate a continuous-medium\* approximation in which the system state is described by a small number of spatio-temporal fields\*, obtained after averaging over the velocities of the system particles (or more generally averaging over kinetic features).

Information: beyond its current meaning, information is associated with a mathematical theory of signal\* transmission and communication channels, developed by Shannon. The central notion is the average information gained through the observation of a discrete-state event or the reception of a coded message:  $I = -\sum_{i=1} p_i \log p_i$  involving the a priori knowledge we have on the event, namely the probabilities  $p_i$  of the possible outcomes i. The information I measures the uncertainty about the outcome (it is rather a "missing" information), being maximal (equal to  $\log N$ ) when all outcomes are equiprobable ( $p_i = 1/N$  for all i) and vanishing in case of a deterministic event ( $p_{i_0} = 1$  for some  $i_0$ ). Note that the log is usually a binary logarithm, so that I is measured in bits.

Instability: spatio-temporal analog of a bifurcation\*, namely a qualitative change in the system spatio-temporal organization when some control parameter\* crosses a threshold. For instance, an homogeneous state turns to develop patterns or traveling waves.

Invariance: it means that the behavior (e.g. statistical properties) of the system is not modified under some transformation acting on the system microscopic state. Invariance is thus closely related to the notion of symmetry\*; for instance, invariance under translations corresponds to homogeneity\*, invariance under rotations to isotropy, and invariance under time reversal to reversibility\*.

Inverse problem: quasi synonym of reconstruction\*; it refers to the issue of inferring the sources and elementary causes from the observation of the system behavior, more often performed at a larger scale and spoiled with the distortions inherent to the experimental setup (e.g. indirect, filtered and averaged measurements).

**Irreversibility:** the existence of a time arrow. An irreversible behavior is any behavior that is not invariant upon time reversal  $t \leftrightarrow -t$ . The puzzle of irreversibility is that Newtonian dynamics (in particular molecular dynamics) is reversible, whereas the observed world is obviously not. The most acknowledged explanation relies on the non-typical nature of the initial conditions in currently observed phenomena (e.g. a drop of ink in water), making highly improbable the reverse evolution.

**Kinetic theory:** mainly developed for dilute gases, this theory deals with the distribution\* functions of positions and velocities. Its central piece is the *Boltzmann equation* describing the evolution of one-particle distribution and involving a decorrelation approximation for closure\* (writing the two-particle distributions as a product of one-particle ones).

**Langevin equation:** stochastic\* extension of an ODE\* dx/dt = F(x) achieved by adding a stochastic force  $f_L$  (or noise\* term) to F(x). The evolution equation now writes  $dx/dt = F(x) + f_L$ . As a result of the cancellations following from the fluctuating nature of  $f_L$ , the random term  $f_L dt$  roughly behaves as  $\sqrt{dt}$ ; it is generally supposed to be fully random (i.e. with no correlations\*) and moreover Gaussian\*, hence fully determined by the knowledge of its first two moments\*:

$$\langle f_L(t)\rangle = 0,$$
  $\langle f_L(t)f_L(s)\rangle = \delta(t-s)A^2(t)$ 

One currently writes  $f_L(t) = A(t)\eta$  where  $\eta$  is a white noise\*. Such a Langevin equation belongs to the more general class of SDE\*.

Originally, Langevin introduced this formalism in the context of Brownian motion; F and  $f_l$  have then the same origin, namely numerous random\* collisions of water molecules on the Brownian particle. F is the coherent contribution building up from these collisions, whereas  $f_L$  is the remaining fluctuating part. Nevertheless, their common origin reflects in the fluctuation-dissipation theorem\*, relating the amplitude of F and the variance of  $f_L$ .

Lattice: discrete counterpart of the real space; it might result from an arbitrary discretization of the continuous space, or reflect some physical reality (crystal lattices, spin lattices).

Limit cycle: periodic solution of a dynamical system; if it is stable, it describes an oscillating asymptotic behavior.

**Linear:** a linear dependence is a mere proportionality. It thus describes only additive\* behaviors, with no collective features. Linear approximation amounts to replace a function\* or a functional\* by its linearized\* counterpart. Linear response theory describes the system response to an external field under the assumption that this response is linear with respect to the field, hence thoroughly characterized by a response coefficient (or a response function  $R(\omega)$  in case of an excitation at frequency  $\omega$ ).

**Linearization:** approximation of a function\* or a functional\* by a linear dependence, corresponding to the first term in its Taylor expansion:  $f(x) \approx f(x_0) + f'(x_0)(x - x_0)$ .

**Lyapunov exponent:** time-average rate of dynamic amplification of infinitesimal errors and disturbances on the system state, in dynamical systems theory. A positive value  $\gamma > 0$  reflects sensitivity to initial conditions and an exponential growth of the separation between two trajectories initially arbitrarily close, thus providing a hallmark of deterministic chaos\*. More explicitly, let  $\delta x(t)$  be the distance at time t between two trajectories initially separated by  $\delta x(0)$ ; then

$$\gamma = \lim_{t \to \infty} \lim_{\delta x(0) \to 0} \frac{1}{t} \log |\delta x(t)/\delta x(0)|$$

It is actually a measure-theoretic quantity, introduced in the framework of ergodic theory and associated with an invariant ergodic\* measure of the evolution; it is shown to be identical for all the generic\* trajectories with respect to this measure.

Macroscopic: (context-dependent) scale of observation; also the highest level in a multi-scale description. It is typically the experimentally accessible level, hence the level of phenomenological models.

**Map:** discrete-time evolution  $x_{n+1} = f(x_n)$  where  $x_n$  is the system state at time  $t_n$  ( $t_n = n\Delta t$ , n-th generation or n-th round in case of varying time step).

Markovian: system whose (stochastic\*) evolution is fully determined by the transition probabilities between two successive times, with no further memory\* of the past evolution.

Maxwell distribution: velocity distribution of a particle of mass m at thermal equilibrium

$$P(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-mv^2/2k_B T}$$

Mean-field: approximation in which a local hence fluctuating\* quantity is replaced by its average\* value over the whole system. It has been originally developed for spin lattices\*: each spin i experiences a local field  $h_i = h(m_i)$  where  $m_i$  is the local magnetization generated by the nearest neighbors of i divided by the number of nearest neighbors, i.e. a magnetization per spin. The approximation is to replace  $m_i$  by its average value  $\bar{m}$  over the whole lattice (i.e. an average over i), thus replacing  $h_i$  by a mean-field  $h(\bar{m})$ . Averaging over the resulting orientations of the spins yields a self-consistent\* equation for  $\bar{m}$ .

**Memory:** extended time dependence in the sense that the knowledge of the system state over a whole time interval (or even the knowledge of its whole history) is required to determine its future evolution. Related issues are on one hand dynamical systems\* with delays, on the other hand aging and hysteresis, e.g. in disordered systems.

Mesoscopic: intermediary scales between microscopic\* and macroscopic\* levels. It is typically introduced through coarse-grainings\* and involves effective\* parameters.

Metastability: transient phenomenon in which a system is trapped in some state, typically a local minimum of its free energy\* or more generally in some phase space region where the dynamics is

highly slowed down. Metastable states nevertheless differ from equilibrium\* states, hence the system will ultimately relax further and equilibrium relations and properties (e.g. fluctuation-dissipation theorem\*) might not apply.

Microscopic: (context-dependent) elementary scale of the system; also the lowest level in a multiscale description. It is typically the level where a theory describing the phenomenon in terms of first principles is available.

**Moments:** statistical averages  $\langle X^n \rangle$  of a random variable X. Irreducible moments (also called cumulants) are defined as the difference between the actual moments and those, denoted  $M_n(m,\sigma)$  of the Gaussian\* variable with the same mean  $m = \langle X \rangle$  and the same variance  $\sigma^2 = \langle X^2 \rangle - m^2$ , i.e.  $\langle X^n \rangle_{irr} \equiv \langle X^n \rangle - M_n(m,\sigma)$ . These irreducible moments quantify the distance to the Gaussian distribution ( $\langle X^n \rangle_{irr} = 0$  whatever  $n \geq 3$  would ensure that X is Gaussian). As can be checked directly, the n-th derivatives in u = 0 of the characteristic function  $\varphi(u) = \langle e^{iuX} \rangle$  and of the generating function  $G(u) = \log \langle e^{uX} \rangle$  are respectively equal to  $i^n \langle X^n \rangle$  and  $\langle X^n \rangle_{irr}$ .

**Multifractality:** extension of the fractal\* geometry to the case of intermingled, superimposed fractal structures. In the most current cases, it refers to the singular structure of a measure or a field  $A(\vec{r})$ , exhibiting in any point a singularity characterized by an exponent  $\alpha(\vec{r})$ , in such a way that the level subsets  $\{\vec{r}, \alpha(\vec{r}) = \alpha\}$  are fractal sets of dimension  $f(\alpha)$ ; this function  $\alpha \to f(\alpha)$  is called the *dimension spectrum* of the multifractal structure.

**Noise:** any influence chosen to be described in an effective\* manner as a random contribution, because it involves (external or lower-scale) degrees of freedom out of reach or chosen not to be described explicitely. A Gaussian noise uncorrelated in time is called a *white noise*. In general, a noise term is not structureless, which reflects in nontrivial distribution and correlation\* function.

**Non equilibrium:** one should distinguish two instances for a system to be in "non equilibrium". It can be *out of equilibrium*, i.e. not yet at equilibrium but in the process of relaxing\* towards a state of equilibrium. Associated themes are slow dynamics, metastability\*, linear response theory\*, self-assembly, and current examples are provided by glasses, protein folding or foams.

It can be far from equilibrium, driven by an external field, or by fluxes in and out at the boundaries, in a steady state with nonvanishing fluxes of matter, energy or charge crossing it. Associated themes are dissipative\* structures and self-organization\*, and current examples are provided by Turing structures, chemical waves or the functioning of a molecular motor.

The frontier between these two notions of non equilibrium is nevertheless not so clear-cut: it refers to the delicate notion of equilibrium\*, which is highly dependent of the context and observation scales.

**Non linearity:** any discrepancy from mere proportionality f(x) = ax in an evolution law dx/dt = f(x) or in the response f(x) to an excitation x. Typical non linearities are associated with a step function f (existence of a threshold), with a polynomial  $f(x) = x^n$ , an exponential  $f(x) = e^{ax}$ , or a sigmoidal shape (accounting for both a threshold and a saturation).

**Order parameter:** any macroscopic observable that reflects quantitatively and if possible also qualitatively (passing from a vanishing to non-vanishing values) the organization or dynamic regime of the system, e.g. the density in a fluid, the magnetization in a magnetic material, the average molecular orientation in a liquid crystal or the radius of gyration of a macromolecule. It is the

quantity on which a phase transition\* or a conformational\* transition is best evidenced.

In *Landau theory* (an example of mean-field\* theory), the free energy\* is directly assumed to be a polynomial function of the order parameter, devised according to the symmetry\* property of the system.

**ODE:** acronym of Ordinary Differential Equation, i.e. a differential equation involving a single variable, say the time t, and a regular differential operator  $\mathcal{D} = \sum_{i=0}^n a_i(t) \ d^i/dt^i$  where  $a_n(t) > 0$ , for which Cauchy conditions of existence and uniqueness of the solution (given the initial condition, i.e. the initial value of the solution and its n-1 first derivatives) are satisfied. Among ODE, dynamical systems are first-order equations dx/dt = F(x). Defining  $x_1 = x, \ldots, x_n = d^{n-1}x/dt^{n-1}$ , it is always possible to transform a one-dimensional ODE of order n into a n-dimensional dynamical system.

Path integral: extension of the finite-dimensional integration (e.g. in  $\mathbf{R}^n$ ) to the case when the integration variable is a function  $f(x) \in \mathcal{F}$  (another name might have been "functional integration"). The central, and delicate, part is to define the measure in the functional space  $\mathcal{F}$  (in plain words, to define the infinitesimal volume element in  $\mathcal{F}$  playing the role of  $d^nx$  in  $\mathbf{R}^n$ ). A well-behaved instance is the case of the Wiener measure over the set of trajectories  $\vec{r}(t)$  of a Wiener process (the mathematical model for Brownian motion) taking advantage of the statistical independence and Gaussian\* statistics of the increments  $\vec{r}(t+dt) - \vec{r}(t)$ .

**PDE:** acronym of Partial Differential Equation, i.e. a differential for a multivariate function, most often a spatio-temporal field\*; it thus involves partial derivatives. Boundary conditions\* play a key role and should supplement the PDE in order to make any statement about the possible solution(s). Fourier or Laplace transformations can be exploited to turn some or all derivatives into algebraic expressions (e.g.  $\partial/\partial t \rightarrow i\omega$  upon a Fourier transformation over time).

**Partition function:** normalization factor  $\mathcal{Z}(T) = \sum_X e^{-U(X)/k_BT}$  involved in the Boltzmann distribution\* of a system (of state X) at thermal equilibrium at temperature\* T. It actually provides a *generating function* whose derivatives give access to several thermodynamic\* quantities. In particular,  $-k_BT\log\mathcal{Z}$  is the free energy\* of the system.

**Percolation:** class of spatially discrete models in which the local state takes only two values 0 or 1. Moreover, the rule in constructing percolation lattices is that the cell states are independent (i.e. no coupling between the cells). Different models can be devised, according to the lattice geometry and to whether the elementary units are lattice cells (*site percolation*) or the links between neighboring sites (*bond parcolation*). The key feature of these models is the existence of a second-order transition for a given value  $p_c$  of the probability p of cell occupancy (the *percolation threshold*) below which only finite clusters (connected sets of occupied neighboring sites) are present whereas connected paths of occupied sites crossing the whole system are present for  $p > p_c$ . Various scaling\* laws and universal\* features can be evidenced at the percolation threshold.

**Perturbation:** slight modification of an equation or evolution law ruling the structure or dynamic regime of a system (or even, if explicitly mentioned, slight applied variation of the system state, e.g. a "perturbation of initial conditions"). *Perturbation approaches* take advantage of the small amplitude of the imposed variation to determine the change in the system behavior as an expansion around the unperturbed solution (it reduces to a linearization\* at lowest order).

**Phase diagram:** partition of the space of control parameters\* into regions associated with different stable equilibrium states (or "phases").

**Phase portrait:** sketch of the flow (ensemble of all trajectories) of a dynamical system\* in its phase space\* (in practice useful only in d = 2).

**Phase space:** the space of possible states of the system under investigation; this space is partly arbitrary since it depends on the description scales and on the amount of details that are retained in the modeling.

**Phase transition:** qualitative change of the overall organization and statistical properties of a system observed when varying a control parameter\* (e.g. the temperature\*, in case of thermal transitions originating in a change in the balance between the ordering achieved by interactions and disorder generated by thermal motions). It is strictly well-defined only in the infinite-size limit  $N \to \infty$  (where N is the number of particles in the system) where it reflects in a singularity\* of the free energy\* at the transition value of the control parameter. The transition is said to be of *first order* if the order parameter\* exhibits a finite jump at the transition, of *second order* if it remains continuous with a singularity in its derivatives. Second-order transitions are a typical instance of critical\* phenomena.

Power law: functional dependence of the form  $Y(x) \sim x^{-\alpha}$  (corresponding to a linear dependence in a log-log plot). The key point is that Y thus varies over an arbitrarily large range, with no characteristic scale (compared for instance to an exponential dependence  $Y(x) \sim e^{-x/a}$  or an oscillating behavior  $Y(x) \sim \cos(2\pi x/a)$  exhibiting a finite characteristic scale a). One speaks of anomalous power law if the exponent  $\alpha$  differs from the value following from plain dimensional analysis (e.g. a fractal\* dimension or an anomalous diffusion\* law  $R^2(t) \sim t^{\gamma}$  with  $\gamma \neq 1$ ). Power laws are the hallmark of critical\* phenomena, exhibiting long-range correlations\*, fluctuations\* at all scales, abnormal response properties (a finite perturbation might generate consequences at arbitrarily large scales). Power-law distributions are a generic\* alternative to exponential and Gaussian\* distributions. They exhibit "long tails", giving a non negligible probability to large events. In case of a small exponent  $\alpha < 3$ , their variance is infinite, which means among other features that rare large events might dominate the observed behavior.

Quasi-static: approximation according which an evolution is described as a succession of equilibrium\* states. It amounts to decouple the fast relaxation\* towards a local equilibrium and a slow evolution of this equilibrium state.

Random: involving a part of chance, e.g. the possibility of several outcomes for the same input. A random event is thus described in a probabilistic framework. Randomness does not preclude some predictability, e.g. if some outcome is more probable than the other ones, or if successive outcomes are correlated\*. Unfortunately, "random" is sometimes used with the implicit additional meaning of "with a uniform probability" and "uncorrelated in time", that should rather be stated explicitly.

Random walk: stochastic\* motion defined as a sequence of statistically independent and identically distributed discrete steps. It provides a mesoscopic\* model of diffusion\*: as soon as the variance  $a^2$  of these steps and their average duration  $\tau$  are finite, the mean-square displacement  $R^2(t) \equiv \langle |\vec{r}(t) - \vec{r}(0)|^2 \rangle$  obeys the normal diffusion law  $R^2(t) \sim Dt$  with  $D = a^2/2\tau$ . Most often, this model is implemented on lattices. Numerous extensions (correlated, self-avoiding, biased, or

confined random walks) can also be considered.

Range: speaking of interactions, it is the distance over which the interaction is noticeable, e.g. the distance a for an interaction potential  $V(r) \sim e^{-r/a}$  or V(r) having a minimum in r=a. A power-law\* dependence  $V(r) \sim r^{-\alpha}$  is said to be long-range (in fact infinite-range). Similarly, the range of correlations\* is the correlation length  $\xi$ , and one speaks of long-range correlations if  $\xi \approx \infty$ .

**Reconstruction:** estimation\* of a model and its parameters from experimental data. In general, additional constraints should be introduced to discriminate between several possible solutions.

**Relaxation:** evolution towards equilibrium, typically after an excitation or starting from non equilibrium initial conditions.

**Renormalization:** different meanings are associated with this term, corresponding to very different status for the associated renormalization procedure.

A renormalized quantity can be plainly a rescaled\* quantity (normalized, dimensionless or put to the scale of the considered sample).

It can be an effective\* quantity accounting in an integrated way or underlying mechanisms of contributions (e.g. the renormalized mass of a body moving in a fluid, accounting for hydrodynamic effects).

Renormalization is also a mathematical technique developed first in celestial mechanics then mainly in quantum electrodynamics to regularize divergent expansions and perturbation\* series. It proceeds by means of resummation, or by introducing a cutoff on the space, time and energy scales, then accounting in an effective way of the host of contributions at smaller space-time scales so as to take advantage from physical cancellation of mathematical divergences\*.

Finally, renormalization also refers to a multi-scale procedure allowing to classify critical\* behaviors, to determine quantitatively critical exponents and to handle associated divergences\*. A renormalization transformation consists in joint coarse-grainings\* and rescalings\*, thus relating two models describing the same phenomenon at different scales; it moreover puts forward their self-similar properties and associated scaling laws, while eliminating specific small-scale details having no consequences on the asymptotic, large-scale behavior. Iteration of this procedure generates a flow in the space of models, whose fixed points correspond either to trivial, either to critical situations (according to their stability). It can be shown that the linear\* analysis of the renormalization transformation around a critical fixed point gives access to the critical exponents. This analysis allows to split the space into universality\* classes, each associated to the basin of attraction of a critical fixed point. The set of renormalization transformations has a semi-group structure with respect to the rescaling factor (or plainly with respect to iteration) and one often speaks of the renormalization group.

Rescaling: multiplication by a given factor of quantities of a given type (e.g. "rescaling of lengths") to get a dimensionless quantity, or to evidence a scaling\* behavior (through the collapse of rescaled data from different systems on a master curve). Joint rescalings of space, time and phase space variables are involved in renormalization\* methods (following a coarse-graining\*) to preserve the size of elementary units composing the system and evidence self-similarity as a fixed-point property.

**Reversibility:** invariance of dynamical equations with respect to time reversal  $t \leftrightarrow -t$ . For ins-

tance, Newtonian dynamics is reversible whereas the diffusion\* equation is irreversible\*.

Robustness: with respect to a certain type of perturbation\*; it means that the observable behavior is qualitatively unchanged under the influence of such a perturbation. Different levels of robustness are to be distinguished according to the nature of the perturbation: robustness with respect to a change in the initial conditions (i.e. *stability*), to a modification of the dynamic equations (i.e. *structural stability*) or to a modification of the model itself (i.e. *universality*).

Scale invariance: extended notion of self-similarity; changing the system size N by a factor of k changes accordingly the value of the order parameter X (or other observables) by a factor of  $k^{\alpha_X}$ . This can be expressed as a scaling law:  $X(kN) \sim k^{\alpha_X} X(N)$ . More generally, scale invariance implies that a dependence between two observables X and Y writes

$$Y(N,X) \sim k^{-\alpha_Y} F(k^{\alpha_X} X, kN)$$
 or  $Y(N,X) \sim N^{\alpha_Y} f(N^{-\alpha_X} X)$ 

This notion can be generalized to any subset of variables, including or not the size N. The notion is specially interesting in case of "anomalous" scale invariance, namely the case when the exponents cannot be determined by a plain dimensional analysis, but build up from a highly correlated internal organization of the system, as in critical\* phenomena.

Scaling: a way of investigating natural systems, focusing on their multiscale architecture, scale-invariant\* properties and the self-similar relations that might exist between different levels. The central role is given to scaling laws, to scaling theories assuming such scaling laws as a basic fact, and to renormalization\* methods. To summarize in plain words, scaling approaches amount to replace a "physics of the amplitudes", aiming at computing the system behavior at a given scale, with a "physics of the exponents", centered on the determination of scaling exponents.

Second Principle: one of the basic principles founding classical thermodynamics\*. One of its numerous formulations is that the (thermodynamic) entropy\* of an isolated system cannot decrease, even transiently. In consequence, any entropy increase, even local and transient, requires an energy exchange with the external world. Microscopic investigations in the framework of statistical mechanics have shown, at least in equilibrium or near-equilibrium situations, that this Second Principle does not state an impossibility (it is currently violated in a system of, say, three molecules) but an improbability due to the large size  $N \to \infty$  of the systems investigated in classical thermodynamics (the same explanation is invoked for the emergence of irreversibility\*).

**Self-consistent:** refers to a general technique used in systems with feedbacks, namely in which some small-scale feature X (a parameter, a field) has consequences at higher levels that exert a retro-action on this very feature. An example is provided by mean-field\* theory encountered for instance in spin lattices: X is here the average magnetization, generating a mean magnetic field h(X) that influences back the spin orientations, hence also the magnetization and its average X. Writing the consistency of this feedback loop yields an implicit equation for the unknown value  $X^*$ , having the form of a fixed-point equation  $f(X^*) = X^*$ .

Another issue is then to solve this equation. A systematic technique is to proceed by iterations:  $X_{n+1} = f(X_n)$ , provided the sequence  $(X_n)_n$  can be shown to converge to  $X^*$  (in particular, it requires an initial condition  $X_0$  enough close to  $X^*$ ).

Self-organization: spontaneous appearance of spatial, temporal or spatio-temporal structures

in a system driven far from equilibrium\* by injection of matter or energy. One also speaks of "dissipative" structures" to underline that dissipation of energy occurs to pay the entropic\* cost of the local increase of order.

Self-organized criticality: systems slowly driven out of equilibrium by a continuous injection of matter or energy might either stabilize in a steady state\* or, in case when some threshold controls the outputs, accumulate this energy or matter up to a situation of marginal stability where it is released in a random\* way, i.e. at random times and during events of random amplitude and duration. More quantitatively, the distributions of the event size, duration and interval typically exhibit a power-law\* dependence, reflecting the absence of characteristic\* size or time, hence a critical\* character. Accordingly, strong long-range correlations\* are present in the structure and dynamics of these systems, and one speaks of self-organized criticality ("self-organized" since the system spontaneous reaches such a regime, without the need of monitoring from outside some control parameter\*). Typical examples are sand or snow piles and their avalanches, earthquakes and landslides, or the inflation of lungs during breathing.

Related situations, involving the same inter-level feedback loops, are those where a dynamic self-tuning of the internal parameters maintains the system in a non generic\* state, e.g. a bifurcation\* point or a critical\* transition point (situations sometimes encountered under the names of "threshold stabilization" or "edge of chaos").

**Signal:** in physics (in contrast to biology), this notion is not endowed with any semantic contents; a signal is simply a time series recorded by an experimental setup.

Singularity: any discrepancy with respect to a smooth behavior, for instance a jump in an otherwise continuous function, a pole in an analytic function, a hole in an otherwise connected region, a cusp on an otherwise differentiable manifold, the divergence\* of a series. Strictly speaking, the singularity is a feature of the mathematical model and not of the real system, in which physical cutoffs or finite-size effects\* always occur at some point and smooth out the singularity, but it nevertheless reflects some actual feature: it is precisely one of the merit of the mathematical formalization to accentuate physical features in such a clear-cut manner.

**Spectrum:** spectrum and accordingly spectral analyses unfortunately refer to a host of different notions, and is to be understood according to the context.

In experimental studies, numerous "spectroscopy" techniques are currently implemented: spectrum then refers to electromagnetic waves emitted or absorbed by the molecules of the investigated sample, thus providing informations on their nature, conformation, interactions, motions and environment. Recently developed techniques of fluorescence spectroscopy now supplement more classical analyses recording e.g. the emission spectra after an excitation (emission of a photon during the relaxation of an excited energy level) or absorption spectra (selective absorption of photons by degrees of freedom, e.g. vibrational, of the system). Techniques are classified according to the frequency range, i.e. energy range of the observed photons, thus probing different features, substructures and degrees of freedom. Spectroscopic studies are the only experimental access to distant objects as stars or interstellars gases.

In signal analysis, one computes power spectra, namely the energy  $S(\omega)$  contained in the component at frequency  $\omega$ . According to the Wiener-Khinchine theorem,  $S(\omega)$  is the Fourier transform of the auto-correlation\* function of the signal.

In any problem whose mathematical formulation involves a linear operator A, the spectrum

refers to the set of complex numbers  $\lambda$  such that  $A - \lambda \mathbf{1}$  is singular, including in particular eigenvalues (for which the kernel of  $A - \lambda \mathbf{1}$  is not reduced to  $\{0\}$ ).

In quantum mechanics, a spectrum is the sequence of energy levels (discrete in its lowest part) of a system. It corresponds to the spectrum of its Hamiltonian, thus matching the mathematical definition of the spectrum of a linear operator. One also recovers the experimental notion of emission or absorption spectrum, since the photons absorbed by the system or emitted after an excitation are associated with a transition between two energy levels, hence have a frequency directly proportional (up to the Planck constant h) to the inter-level spacing of the energy spectrum.

Finally, the term spectrum might be used almost in its current meaning of "range", "sampling", "distribution". For instance, in proteomic analyses, the *mass spectrum* of a protein mixture is the sequence of masses of the different molecules present in the sample, allowing by a one-to-one relation to identify its composition.

**Stability:** feature of an equilibrium\* state, according which any small perturbation of this state relaxes\* to 0 (exponentially fast). In case of a dynamical system dx/dt = V(x) with an equilibrium state in x = 0, i.e. V(0) = 0, the stability is determined by the sign of the real part of the eigenvalues of the Jacobian matrix DV(0) (all should be strictly negative).

Statistical mechanics: microscopic theory of many-body systems aiming at determining their macroscopic\* properties from first principles (thermal motion and molecular interactions). This goal is achieved provided one restricts to statistical properties. The central piece is the ergodic\* hypothesis and ensuing Boltzmann\* distribution, allowing to circumvent a molecular dynamics study (by contrast to the kinetic\* theory) and to perform the whole analysis in the configuration space. It successes range from providing a microscopic support to thermodynamics\* up to explaining critical\* phenomena, when supplemented with renormalization\* methods. Within a linear\* framework (linear response theory), it has been extended to near-equilibrium situations. Work is still in progress for far from equilibrium systems (a direction is to use notions and tools from dynamical systems\* theory and chaotic\* dynamics).

**Steady state:** stationary state differing from an equilibrium state in that fluxes of matter, charge or energy cross the system.

**Stochastic:** a synonym of random\*, more specifically used for time evolution involving some randomness in its updating rules (e.g. one speaks of "random variables" and "stochastic processes"). The associated evolution law is given in a probabilistic framework. Stochastic convergence, stochastic calculus and stochastic integration refer to the extension to stochastic processes, developed in a measure-theoretic framework, of usual notions of convergence of a sequence, differential calculus and integration theory.

**Structural stability:** a dynamical system is said to be structurally stable when its asymptotic\* features remain qualitatively unchanged upon a small perturbation\* of its evolution\* law. This property will depend on the space in which perturbations are chosen and on its topology (giving a quantitative meaning to the smallness of the perturbations).

**Sub-additivity**: property of a function according which  $f(x+y) \leq f(x) + f(y)$ . It ensures the existence of a finite limit:  $\limsup_{x\to\infty} f(x)/x < \infty$ .

Symbolic dynamics: it is possible to reduce a discrete-time dynamical system\* to a symbolic

formulation by introducing a suitable finite partition  $(A_{\omega})_{\omega=1...k}$  of the phase space\*: the system state  $x_t$  at time t is coded by the label  $\omega_t$  is  $x_t \in A_{\omega_t}$ . Trajectories are thus represented by symbolic sequences  $(\omega_t)_{t\geq 0}$ . The point is that for generic\* chaotic\* dynamics, this coding involves no loss of information: knowing the sequence  $(\omega_t)_{t\geq 0}$  thoroughly determines  $x_0$ , hence the ensuing trajectory. Moreover, a quantitative estimation of chaotic\* features, e.g. Kolmogorov-Sinai entropy, can be done on this symbolic representation of the dynamics. More generally, one merit of such a symbolic representation is to put forward universal features of the dynamics.

**Symmetry:** invariance \* of the system upon some transformation (for instance translations, rotations or time-reversal). A symmetry might be discrete (a periodic structure is invariant upon translations of length equal to an integer multiple of the period) or continuous. It might be exact or only statistical, i.e. satisfied by the average properties or the distribution functions.

Symmetry breaking is a situation where the observed behavior is less symmetrical than the laws and equations ruling it: let us cite for instance the spontaneous appearance of a periodic pattern while initial composition and mechanisms at work in the system are homogeneous.

**Temperature:** intensive variable defined in the framework of thermodynamics\* (zeroth law): two bodies in equilibrium\* (in contact each with the other, and after a time enough long so that no observable change in the bodies state can be detected macroscopically) have the same temperature. It can be formally defined once assumed the existence of thermodynamic entropy\* S: denoting U the internal energy,  $(\partial S/\partial U)_{V,N} = 1/T$ . As such, it plays a central role in heat and work exchanges (Carnot cycle, thermostats, Second Principle, heat equation and the Fourier law, to cite but a few main themes of classical thermodynamics). It has been given a microscopic meaning and role with the development of statistical mechanics\* and kinetic theory\*. At equilibrium\*, the average\* kinetic energy of a particle is  $3k_BT/2$  where  $k_B$  is the Boltzmann constant and its velocity distribution is the  $Maxwell\ distribution$ 

$$P_M(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-mv^2/2k_B T}$$

More generally, the equipartition theorem ensures that any degree of freedom is endowed with the same energy  $k_BT/2$  (the characteristic thermal energy) at thermal equilibrium. The temperature is also involved in the Boltzmann distribution, describing the relative weight in the configuration space of the system, reflecting quantitatively the balance between thermal and potential energies:

$$P_T(X) = \frac{1}{\mathcal{Z}(T)} e^{-U(X)/k_B T}$$

The inverse temperature  $\beta = 1/k_BT$  (the inverse of an energy) is frequently used instead of T.

Thermodynamic: refers to macroscopic and phenomenological variables, relations or arguments, as those involved in classical thermodynamics. The four principles founding thermodynamics are the zeroth-principle (equality of equilibrium temperatures of two bodies in contact), first principle (energy conservation), second principle (increase of the entropy of an isolated system) and third principle (vanishing of the thermodynamic entropy extrapolated at zero temperature). Concretely, one assumes the existence of a state function S(U, V, N) depending on the volume V, the particle number N and internal energy U, whose derivatives yield thermodynamic quantities, e.g. the temperature through  $(\partial S_{th}/\partial U)_{V,N} = 1/T$ . Advances in statistical mechanics\* provided a micro-

scopic basis to thermodynamics of equilibrium\* states and linear\* reponse theory; an analogous microscopic support for thermodynamics of irreversible processes is still lacking.

Universality: in the context of critical phenomena\*, universality refers to the fact that seemingly very different systems (e.g. a fluid and its liquid-vapor phase transition\*, or a magnetic material and its ferromagnetic transition) exhibit the same critical behavior, in particular their critical exponents are exactly equal, thus defining universality classes of critical phenomena. Renormalization\* studies have shown that universality classes of thermal transitions were prescribed by only two geometric parameters: the space dimension d and the number n of components of the order parameter\* of the transition. In more general instances, universality classes can be determined as the basin of attraction of a critical fixed point under the action of a suitable renormalization group.

Variational methods: formulation of a problem in such a way that its solution  $X^*$  appears to minimize some functional\*  $\mathcal{F}(X)$  (possibly under additional constraints):  $\delta \mathcal{F}(X^*) = 0$ . This endows the considered problem with a geometric interpretation: a landscape  $\mathcal{F}(X)$  whose relief leads to the solution  $X^*$  when following valleys and steepest-descent paths.

Wavelets: a method of signal processing providing a local and multi-scale generalization of Fourier or Laplace transformations. By performing a convolution of the signal with a localized kernel (a "wavelet" w(t) of bounded support), rescaled by a factor b and translated at time  $t_0$ , one obtains the contribution  $S(b,t_0)$  of the wavelet at scale b and time  $t_0$  to the signal. The wavelet might be chosen to resemble inherent patterns of the signal, in order to minimize the number of relevant contributions. The resulting decomposition can be seen as the "music score" corresponding to the original signal: a sequence of notes, i.e. prescribed frequencies, played at prescribed instants, over a prescribed duration.

White noise: Gaussian\* noise\* uncorrelated in time. It is fully determined by its first two moments\*:

$$\langle \eta(t) \rangle = 0,$$
  $\langle \eta(t)\eta(s) \rangle = \delta(t-s)$