Research Interests

My research activity has been always related to computational physics of many body systems, in particular it has been focused along the following research lines:

1) Nonlinear dynamics and statistical mechanics of many body systems out of equilibrium

2) Microscopic dynamics of simple and molecular liquids

The first topic has been the subject of my Laurea thesis, while the second one of my Ph.D. thesis. In the last six years, my activity has been focused mainly on the first topic and also my future research will mainly concern complex systems with many degrees of freedom.

To be more specific I am at the moment studying the dynamical behaviours and the phase transitions of systems out of equilibrium employing both computational approaches as well as theoretical ones. The dynamics of such systems is characterized with standard indicators (e.g. correlation fuctions, distribution functions, escaping times, distribution momenta etc.) as well as adopting chaotic indicators (e.g. Lyapunov exponents or fractal dimensions). The models studied are usually N-body systems interacting with short or long ranged forces and they range from chains of coupled nonlinear oscillators (e.g. the Fermi-Pasta-Ulam model) and PDE's equations exhibiting spatio-temporal chaotic behaviours (e.g. the complex Ginzburg-Landau equation), to toy models designed to mimic the folding dynamics of etheropolymeric chains.

More in detail I am actually involved in the following research activities, that I will pursue also in the next years :

a) Dynamical and statistical approach to the protein folding problem: coarse-grained models in 2d and 3d are considered, these models are introduced to mimick the main features of the protein folding phenomenon observed in real systems. From a statistical point of view, we would like to characterize the folding transition in terms of a Markovian process on a tree connecting subsequent metastable configurations separated by free energy barriers. The passage from one configuration to another is supposed to be describable in terms of an activation process. Our claim is that "good folders" are connected via many different pathways to the native state, while "bad folders" and homopolymers are connected to the minimal energy configuration via an extremely limited number of pathways. This difference should explain why good folders reach the native state on time scales much shorter than the bad folders. Preliminary studies in this directions have been pursued cosidering a 2d model recently introduced by Stillinger et al. (1993), and a first analysis confirms our claims. From a dynamical point of view, we have characterized the folding dynamics of various sequences, observing peculiar characteristics in the time evolution of good folders that distinguish clearly them from bad folders. We would like to extend these studied to more realistic 3d models in order to compare our numerical results with experimental data. In collaboration with L. Bongini, R. Livi, and A. Politi (Firenze - Italy). **Related Pubblications : 50** (see the enclosed pubblication list)

b) Study and characterization of the transitions from phase turbulent to defect turbulent regime observed for the 1d, 2d and 3d complex Ginzburg-Landau equation (CGLE), with particular emphasis on the role played by particular exact solution of the CGLE (termed modulated amplitude waves (MAW's)) in the phase turbulent regime and on the mechanism leading to defect formation. Recently. MAW's have been observed in various experiments on hydrothermal waves: namely, in annular convection channels (Janiaud et al. (1992) and Mukolobwiez et al. (1998)) and in linear convection cells (Garnier et al. (2001)). Moreover, recent experimental observation of MAW's have been reported for a Taylor-Dean system (Bot et al. (2000)) and also in a 2d oscillatory variant of the Belousov-Zhabotinsky reaction in connection with the occurence of the so-called "super-spirals" (Ouyang et al. (2000)). In collaboration with the Ouyang's group we are presently investigating the origin of the super-spirals breakup, leading to defect turbulence, in a 2d variant of the CGLE. Due to the relevance of the MAWS's for the experimentalists, we are planning to extend our investigation on the stability and existence of MAW's also to more realistic systems, like the Oregonator or the FitzHugh-Nagumo equation, In collaboration with M. Baer and L. Brusch (Dresden-Germany), M. van Hecke (Leiden-The Netherlands) and M.G. Zimmermann (Argentina). **Related Pubblications : 27,28,31,43,46,49**

c) Study of the thermodynamics and dynamics of self-gravitating models : these are Hamiltonian models with long-range Newtonian-like interactions. N-body hamiltonian systems with long range forces reveal several interesting phenomena, such as clustering and anomalous relaxation to the equilibrium. In some of these models the dynamics of the single particle depends self-consistently on the time-behaviour of "mean-field" quantities, obtained averaging over all the particles of the system (Antoni and Ruffo). Such self-consistent dynamics lead to clustering and de-clustering phenomena that can be related to a second order phase transition in the system. In 2 dimensions we have shown that the clustering transition is first order and that it is related to anomalies in the thermodynamics of the system (e.g. a region of "negative specific heat" has been observed near the transition) as well as in its dynamical behaviour: diffusion of particles in these systems is not ruled by usual Brownian motion. But a competition of localized and ballistic behaviours instead leads to anomalous diffusion. Some preliminary indications suggest that these motions can be interpreted within the class of the Levy-walks. Moreover, the observed superdiffusive behaviour is clearly related to the existence of a clustered state. For the first time a transition from a clustered to a homogeneous state has been related to a dynamical transition from anomalous to ballistic motion. We are presently working on a generalization of the previous model in 2d, this new model depending on a parameter is able to exhibit both first and second order clustering transitions. In particular, we are observing that a negative specific heat regime is present only in connection with first order transitions. We plan to investigate in more details these findings due to their relevance not only for the statistical mechanics community but also for the astrophysicists. Moreover, we would like to extend such studies to more "realistic" models of self-gravitating systems (e.g. to three dimensional models). In particular, we are interested to understand if the connection between thermodynamical anomalies and anomalous diffusion still holds in more physical systems. In collaboration with M. Antoni (Marseille - France) and S. Ruffo (Firenze - Italy). **Related Pubblications : 35,41,44**

A more detailed description of all my past and present research activity, as well as copies of my pubblications, can be found on my personal web page:

http://www.ino.it/~torcini