Project achievements

WP1: Complex network: theory, simulations, applications.

- Studying properties of multicomponent molecular networks/gels with applications to liquid crystals. This includes elaborating and studying by computer simulation methods coarse-grained models describing the dynamics of formation and equilibrium structural properties of multicomponent gels, in particular, photo-controllable gelation of gold nanoparticles decorated by azobenzene groups. As a result, the wall-to-wall percolation (and hence forming a network) was described in both pure liquid crystalline elastomer (LCE) systems and in LCE systems doped by nanoparticles.
- Explaining the universal shape characteristics for the mesoscopic polymer chain immersed in different solvents. In particular, universal shape characteristics for the mesoscopic polymer chain immersed in solvents of different nature was examined and explained using the mesoscale simulation approach to the dissipative particle dynamics.
- Contributing to the theory of star-like polymers in solvents and micelle formation. This includes studying scaling properties of the shape characteristics of a number of configurations of polymers (linear chain, single homo- and star-polymer) by means of a mesoscopic modeling approach to the dissipative particle dynamics. This also includes micellization of the solution of amphiphilic star-polymers in a solvent of variable quality and thus obtaining the dependence of the size and the form of micelles on the aggregation number, with possible extension to drug delivery related cases.
- Contributing to the theory of irregular and random graphs and networks by studying properties of Gibbs random fields on such structures. This includes studying Gibbs states of spin models on hierarchical random graphs, on annealed scale-free networks and complete graphs. In particular, location of the Lee-Yang and Fisher zeros of the partition functions of such models.
- Developing a complex-network approach to visualizing and quantifying the evolution of scientific topics, that includes also methods of evaluating the reaction of the scientific community to urgent topics that abruptly arise. Elaborating new cryptographic systems over arithmetic rings based on the idea of hidden discrete algorithms.
- Contributing to the theory Gibbs states of classical models on random geometric graphs. In particular, developing a mean field theory of phase transitions in the Potts model with invisible states, introducing and studying two models of continuum systems of point particles that manifest a liquid-vapor phase transition. Also studying quenched Gibbs states of classical magnets residing on stochastic point processes.
- Contributing to the development of the mathematical theory of states of thermal equilibrium of infinite systems of quantum anharmonic oscillators (quantum crystals). The main concept of this theory is to describe local states in terms of stochastically positive KMS systems and path measures. The global states are constructed as Gibbs path measures satisfying the corresponding DLR equation. The multiplicity of such measures is then treated as the existence of phase transitions.
- Contributing to the theory of quantum systems with deformed commutation relations. This includes studying two-level *q*-deformed Bose systems by locating the zeros of the correlation functions and the Fisher zeros of the partition of this system. This also includes developing various aspects of the theory of quantum particles with non-commutative coordinates and momenta. In particular, the influence of the non-commutativity on the energy levels of the hydrogen atom was studied in a rotationally invariant noncommutative phase space.

WP2: Microscopic modeling in spatial and evolutionary biology.

- A general mathematically rigorous and practically useful framework has been elaborated that might be widely applicable in individual-based modeling of animal movement, as well as in other problems of theoretical ecology. By formulating a unified framework for a wide class of models we developed methods that yield closed system of equations whose solutions give the next term of the approximation beyond the mesoscopic limit. The study was performed of the equations describing the spatial logistic model and its generalization towards including dispersion spreading and monostable reactions.
- An individual-based model of an SIS system on a random graph has been proposed, validated and studied by analytic and computer simulation methods. Various aspects of its dynamics, steady states and spatial patterning were studied. A more advanced version of this model is the SEIS model which we also introduced. In this model, the agents can also be in the exposed state. For this model, we performed the same study and obtained results that lead to general conclusions towards individual-based modeling of the spread of infections and similar phenomena in random environment.

WP3: Microscopic (Markov) dynamics of continuum particle systems with applications.

- The Markov dynamics of infinite systems of point particles in the continuum was described. The Markov generators of various types were studied, including those describing jumps with attraction and repulsion, coagulation, fragmentation, birth-and-death processes, multi-type particle systems, etc. In particular, the dynamics of a spatial ecological model was described in which the constituent entities reproduce themselves at distant points (disperse) and die with rate that includes a competition term. The role of the tradeoff between the dispersal and competition in such systems has been revealed. The Markov evolution of states of a continuum migration model was also described. The model is an infinite system in which the constituents reside on a continuous space, immigrate to this space with state dependent rate and emigrate from it due to competition. A method of identifying the evolution of states of an infinite particle system from the evolution of holomorphic functionals was elaborated. A number of new properties of holomorphic maps of infinite-dimensional Banach spaces were proved to hold, and the study of the iterates of such maps in complex Banach spaces was conducted.
- A general approach to studying the statistical mechanical properties of interacting particle systems was developed that employs considering the system at different hierarchical levels. The basics of the analysis on configuration spaces and *p*-adic spatial combinatorics were elaborated. The *p*-adic theory of the motion in porous random medium was developed. By means of generalizations of the Hausdorff measures and dimensions, fine fractal properties of the probability measures as systems' states were described.

WP4: Meso- and macroscopic dynamics of continuum particle systems with applications.

- A unified approach is proposed to describing the statistics of the short-time dynamics of multiscale complex systems. The probability distribution of the relevant time series (signal) is represented as a statistical superposition of a large time-scale distribution weighted by the distribution of certain internal variables that characterize the slowly changing background.
- By means of convolutional derivatives the dynamics of interacting particle systems was described. By a subordination principle the kinetic fractional dynamics was constructed in

terms of the solutions of Vlasov-type hierarchies. Conditions for the intermittency of the fractional kinetic dynamics to appear were obtained.

- There was studied the stability of stationary solutions for a class of nonlocal semi- linear parabolic kinetic equations. Sufficient conditions were found for the asymptotic stability of the zero solution to hold which was then used in the study of the spatial logistic equation of population ecology. Accelerated propagation of solutions to kinetic equations with a nonlocal linear dispersion on the real line and monostable nonlinearities were found.

WP5: Compartmental models with time delays and stochasticity.

- A general mathematical framework for individual based models (IBMs) containing interactions of an unlimited level of complexity was elaborated and equations that reliably approximate the effects of space and stochasticity were derived. We provided software, specified in an accessible and intuitive graphical way, so that any researcher can obtain analytic and simulation results for any particular IBM. We illustrated the framework with examples from conservation biology and evolutionary ecology.
- A number of IBMs describing infectious disease spread were studied. This includes models based on massive datasets obtained recently during pandemic spread of some viral diseases.

WP6: Mathematics and physics of the evolution of complex shapes.

- An approach was elaborated that allows for constructing new processes of Stochastic Löwner Evolution (SLE) type that possess conformal invariance and the domain Markov property. We gave a Hamiltonian formulation of the evolution of shapes and provided conservation laws based on the Löwner-Kufarev equation. We constructed coupling of the Gaussian free field with slit holomorphic stochastic flows which contains known SLE processes (chordal, radial, and dipolar) as particular cases.
- We developed a version of the conformal field theory based on the background charge and Dirichlet boundary condition modifications of GFF and present martingale observables for these types of SLEs. A model of intermittency is presented in which the dynamics of the rates of energy transfer between successive steps in the energy cascade is described by a hierarchy of stochastic differential equations. Numerical simulation of the general SLE was developed and implemented by using Wolfram Mathematica software.

WP7: Geometry of the space of shapes and pattern recognition.

- The space of shapes an infinite-dimensional manifold of smooth curves was studied by means of methods of the conformal evolution deforming the unit circle.