Publishable summary:

The scientific aim of the project is to make a major step forward in developing effective mathematical tools for studying complex systems based on stochastic geometry and stochastic evolution. The studied system are supposed to consist of large (infinite) number of interacting entities and may evolve in space and time. Both their structure and evolution are of interest. Such systems are studied in broadly understood statistical physics, ecology, population biology, epidemiology, etc. The planned research tasks are divided into seven working packages (WPs). During the realization of the project, the following progress was achieved.

WP1: Complex network: theory, simulations, applications.

The package is aimed at studying complex networks, polymers, liquid crystals, irregular and random graphs, Gibbs random fields on such graphs, quantum systems. Herein, we have achieved the following.

- Properties of multicomponent molecular networks/gels with applications to liquid crystals: (a) coarse-grained models were developed for studying the dynamics of formation and equilibrium structure properties of multicomponent gels; (b) photo-controllable gelation of gold nanoparticles decorated by azobenzene groups was simulated and its dependence on the concentration of nanoparticles was analyzed; (c) for the patchy-decorated gold nanoparticles, the role of the patching pattern was clarified, including the properties of the resulting gel structure, especially its mechanical stability important in applications.
- Theory of star-like polymers in solvents and micelle formation: (a) scaling properties of the shape characteristics of a linear chain, as well as of a single homo- and star-polymer, have been studied using mesoscopic modeling approach of dissipative particle dynamics; (b) micellization of the solution of amphiphilic star-polymers have been performed in a solvent of variable quality resulting in obtaining the dependence of a size and a form of micelles on aggregation number, with possible extension to drug delivery related cases.
- Theory of irregular and random graphs and networks: A number of new results in the theory of Gibbs states of spin models on annealed scale-free networks and complete graphs were obtained. Among them the location of the Lee-Yang and Fisher zeros of the partition function.
- Scientometric and cryptographic applications: A complex-network approach was developed 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; new cryptographic systems were proposed over arithmetic rings based on the idea of hidden discrete algorithms.
- Gibbs states of classical models: A mean field theory of phase transitions in the Potts model with invisible states was developed. Two models of continuum systems of point particles were proposed and studied, that includes also describing liquid-vapor phase transitions in both ones. Quenched Gibbs states of continuum classical magnets are constructed and the existence of magnetic phase transitions in these magnets was proved.
- Gibbs states of quantum models: The basic elements of the mathematical theory of states of thermal equilibrium of infinite systems of quantum anharmonic oscillators (quantum crystals) were developed. The main concept of this theory is to describe local states in terms of stochastically positive KMS systems and path measures.
- Quantum systems with deformed commutation relations: Time-dependent correlation functions of a *q*-deformed Bose gas were studied. A particular case of the two-level *q*-

deformed Bose system is examined and the zeros of the correlation functions and the Fisher zeros of the partition function are analyzed. Various aspects of the theory of quantum particles with non-commutative coordinates and momenta were developed. 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.

The package is dedicated to the individual-based modeling in spatial biology. In this direction, we have achieved the following.

- Microscopic models of animal movement in random media: 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.
- Describing population dynamics as Markov evolution in random media: Here we mostly concentrated on studying models of infectious disease spread. 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, in which the agents can also be in the exposed state. For this model, we have performed the same study. The results obtained for both models 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 package is dedicated to the development of a microscopic dynamical theory of interacting point entities distributed over continuum space and evolving in time. Such systems are studied in physics and life sciences. In their studying we have achieved the following.

- Identifying Markov generators and studying the corresponding dynamics: The Markov dynamics of infinite systems of jumping point particles was described. The generators of various types were studied, including the cases of coagulating jumps and of multi-type systems (Widom-Rowlinson model). 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 immigrate with state dependent rate and disappear emigrate, also due to competition.
- Further generalizations, deriving a priori information on the behavior of the processes: 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 basis of the analysis on configuration spaces and *p*-adic spatial combinatorics was 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. General aspects of the ergodic theory in applications to the studied systems were developed.

- Studying holomorphic generating functionals: 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.

WP4: Meso- and macroscopic dynamics of continuum particle systems with applications. The package is aimed at deriving meso- and macroscopic description of the dynamics of particle systems from their microscopic study. Here we have achieved the following.

- Mesoscopic scaling of microscopic Markov evolutions: A scaling procedure was elaborated and applied that combines features of Kac, Vlasov and some other scaling techniques. By means of convolutional derivatives the dynamics of interacting particle systems was described. By a subordination principle the kinetic fractional dynamics in terms of the solutions of Vlasov-type hierarchies was constructed. Conditions for the intermittency of the fractional kinetic dynamics to appear were obtained.
- Hydrodynamic evolution: A unified approach is proposed to describe 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.
- Front propagation, invasion, homogenization, pattern formation and long-time asymptotic: There was studied the stability of stationary solutions for a class of nonlocal semi- linear parabolic 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 equations with a nonlocal linear dispersion on the real line and monostable nonlinearities were found.

WP5: Compartmental models with time delays and stochasticity.

The package is aimed at developing compartmental individual-based modeling (IBM) of infectious disease spread. Here we have achieved the following.

- Principles and techniques for studying compartmental IBM with possibly non-Markovian residence time: A general mathematical framework for 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.
- Revisiting and studying **c**lassical and recent models of mathematical biology: A number of IBM 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.

In this direction, we have achieved the following.

- Gaussian Free Field approach to non-perturbative minimal models of the field theory:

An approach was elaborated that allows for constructing new processes of Stochastic Löwner Evolution type that possess conformal invariance and the domain Markov property.

- Construction of homotopies by means of deterministic Löwner and Löwner-Kufarev evolutions and their stochastic counterparts:
  We gave a Hamiltonian formulation of the evolution of shapes and provided conservation laws basing on the Löwner-Kufarev equation.
- Coupling GFF and the stochastic shape evolution, construction of the corresponding observables:
  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.
- Relation of different interface evolutions and exactly solvable models:
  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.
- Computer simulation of evolutions of random and deterministic interfaces:
  Numerical simulation of the general SLE was developed and implemented by using Wolfram Mathematica software. We described the applied method together with some technical difficulties, which motivates the structure of the program.

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

In this direction, we have achieved the following.

- Shapes as an infinite-dimensional manifold of smooth curves, probabilistic models of shapes:
  The space of shapes was studied, applying the methods of the conformal evolution, deforming the unit circle.
- Elaboration of sub-Riemannian geometry and geometric control with constrains, controllability in the space of shapes, shape tuning: We describe a graph parametrization of rational quadratic differentials with presence of a simple pole, whose critical trajectories form a network depending on parameters focusing on the network topological jumps. The obtained bifurcation diagrams are associated with the Stasheff polytopes.
- Applications to computer vision and to neurogeometry: The metric approach to studying 2-step nilpotent Lie algebras by making use of non-degenerate scalar products was realized.
- Elaboration of algorithmic and statistical procedures to perform computer simulation of shapes: We constructed a method of numerical simulation for (δ,σ)-Löwner chains.