General progress of the project

2. Qualitative indicators of progress as successes in line with workplan and milestones

In the text below, by writing [I,X] (resp. [II,X]) we refer to the corresponding item of the first (resp. second) part of the list of publications.

During the realization of the project, the following progress was achieved:

Work Package 1. Complex network: theory, simulations, applications.

Task 1.1: Developing coarse-grained models for percolation-related phenomena in pure LCE, LCE doped by non-spherical nanoparticles and copolymer melts.

A coarse-grained model for the liquid crystalline elastomer (LCE) doped by gold nanoparticles has been developed in [I,62]. Since the applications range from solar cell technology (focusing on charge transport in such media) to heterogeneous catalysis, the model is chosen to be general enough to describe these and related features. Namely, gold nanoparticles are supposed to be decorated by ligands of variable length that are terminated by a liquid crystalline group. To cover the case of photo-controllable gelation the option is included for the liquid crystalline groups to represent azobenzene chromophores. The dimensions of all the components are based on real materials, namely the nanoparticles of 2-5nm, alkyl spacer chains and the dimensions of the azobenzene group. The solution of decorated nanoparticles of various concentration is considered in a slit-like pore with its walls decorated by a layer of frozen particles to represent a solid wall. The model is aimed at studying the wall-to-wall percolation in both LCE systems doped by nanoparticles and the ones without these.

Tasks 1.2 and 1.3: Studying the dynamics of network formation and the structure of equilibrium morphologies, their network structure; studying percolation and related properties of the network by corresponding mathematical tools.

In [I,61] and [I,62], by computer simulations the dynamics of network formation has been studied in the following two cases. The first case comprises the photo-controllable network of nanoparticles that are characterized by a longer ligand length (4 coarse-grained beads roughly equivalent to 12 hydrocarbon units) terminated by the azobenzene group. Such scenario was discovered in a recent experimental study [L. Lysyakova et al. J. Phys. Chemistry C 119, 3762 (2015)]. The simulations were performed to mimic a polar solvent which under visual light promotes formation of physical crosslinks between decorated nanoparticles and hence the formation of a network. By applying the UV illumination, azobenzenes switch to a polar cis form breaking the links and turning the solution into a colloidal dispersion. The simulations were performed in a series of “on-off” pulses (with respect to the UV illumination) with 10ns duration of each “on” and “off” part, 10 pulses in total. The properties of resulting network was examined based on the number of subnetworks being formed, average and maximum subnetwork size and maximum network wall-to-wall span. It was found that the network possess the best percolating abilities at the concentrations being about half of the concentration at which the solution turns into a melt with no solvent being present. At higher concentrations that that we observe the competition between the aggregation of decorated nanoparticles and their bulk self-assembly. The second case comprises a wide range of patchy decorated nanoparticles by the use of shorter ligands of 2 coarse-grained beads (approximately 6 hydrocarbon groups) and an ordinary liquid crystalline group [II,28]. Patching patterns with different spatial symmetry were used, namely the uniaxial, three- and four-fold planar, uniform equatorial, icosahedral-based and symmetric axial. It has been demonstrated that the dynamics of the network formation is strongly dependent on the decoration pattern. Typical time for the model to form a network is of order of 10 ns. Simulation results reveal that temporally stable networks are formed by more spatially symmetric decoration patterns, in particular the one comprising six patches of two ligands each located symmetrically along each spatial axis. In total from 5 to 10 attempts of network formation was performed. The simulations indicate that the stable percolation is achieved for certain decoration patterns only, namely the ones with 3,4 and 6 patches of ligands and with equatorial decoration. The network structure for each case being considered is analyzed by a set properties, namely: the maximum subnetwork (giant component) size S_{max} and the wall-to-wall span Z_{max} average vertex rank K and local clustering coefficient C and effective wall-to-wall spring constant E of the network. The spring constant E characterizes mechanical stability of the network and is of particular interest for the applications in heterogeneous catalysis using gold nanoparticles gel systems [V. Ramtenki et al. Coll. Surf. A 414, 296 (2012), Y. Che et al., J. Coll. Interf. Sci. 445, 364 (2015), X.-Q. Wu et al. Appl. Surf. Sci. 331, 210 (2015)].

Task 1.4: Describing universal features of complex polymer networks and Gibbs states on regular and irregular structures.

1.4.1 Explaining the universal shape characteristics for the mesoscopic polymer chain immersed in solvents of different nature:

In [I,66], the universal shape characteristics for the mesoscopic polymer chain immersed in solvents of different nature have been examined using the mesoscale simulation approach of dissipative particle dynamics. It was shown that for the chain lengths N>10, not only the end-to-end distance and gyration radius but also all the three eigenvalues of the gyration tensor scale with the same power law. The Flory exponent ν obtained for each of these properties independently, within the accuracy of the simulations, is close to the best theoretical estimate ν=0.588. Following the analytic expressions, the simulation results for the shape characteristics of the chain were found to be independent of N in the same interval of chain lengths. For the skewed probability distributions of shape characteristics, the heuristic analytic expressions were suggested based on the Lhuillier form (the one derived previously for the radius of gyration of a polymer chain). For the symmetric distributions of other shape characteristics, a generalized Gaussian distribution was used. This allowed to leads to simple analytical expressions with the coefficients and exponents found from fitting the simulation data. This allowed to complement the mean values for the shape properties by their most probable values found as the maximal positions of the respective distributions. The study has been generalized to the case of a star-like polymer in solvents of various quality, see [II, 29]. The dissipative particle dynamics simulations were performed for the homogeneous and four different heterogeneous star polymers with the same molecular weight. The gyration radius and asphericity at the poor, good and θ-solvent regimes were analyzed. Detailed analysis based on the interplay between the enthalpic and entropic contributions to the free energy of the asphericity of individual branches was given to explain the increase of the asphericity in θ-solvent regime, see [II,30]. In particular, at the θ-point condition, the enthalpic contribution vanishes and the branch conformation are driven exclusively by the entropy. This provides means for the wider spectra of possible conformations from collapsed to the coiled ones. This explanation was checked by the analyses of the asphericity of the individual branches by observing the two-maximum shape for their distribution near θ-condition. This confirms the coexistence of two types of conformation, namely, more coiled and more collapsed ones near the θ-point.

1.4.2 Partition function zeros analysis for the Gibbs states of the Ising model on complete graphs and on annealed scale-free networks:

The partition function of the Ising model on graphs of two different types (complete graphs and annealed scale-free networks for which the degree distribution decays as power law with decaying exponent λ) had been analyzed. We were interested in zeros of the partition function in the cases of complex temperature or complex external field (Fisher and Lee-Yang zeros respectively). For the model on an annealed scale-free network an integral representation for the partition function had been found. It reproduces the zeros for the Ising model on a complete graph in the case $\lambda > 5$. For $3 < \lambda < 5$ we derived the λ-dependent angle at which the Fisher zeros impact onto the real temperature axis. This, in turn, gives access to the λ-dependent universal values of the critical exponents and critical amplitudes ratios. Our analysis of the Lee-Yang zeros reveals a difference in their behavior for the Ising model on a complete graph and on an annealed scale-free network when $3 < \lambda < 5$. Whereas in the former case the zeros are purely imaginary, they have a nonzero real part in latter case, so that the celebrated Lee-Yang circle theorem is violated, see [I,85], [I,86], [I,55], [II,43].

1.4.3 Scientometric analysis of the evolution of scientific topics via the case study of the reaction of the academic community to the Chornobyl disaster:

The reaction of academic communities to a particular urgent topic which abruptly arises as a scientific problem had been analyzed. To this end, we have chosen the disaster that occurred in 1986 in Chornobyl (Chernobyl), Ukraine, considered as one of the most devastating nuclear power plant accidents in history. The academic response is evaluated using scientific-publication data concerning the disaster using the Scopus database to present the picture on an international scale and the bibliographic database "Ukrainika naukova" to consider it on a national level. We measured distributions of papers in different scientific fields, their growth rates and properties of co-authorship networks. The elements of descriptive statistics and the tools of the complex network theory are used to highlight the interdisciplinary as well as international effects. Our analysis allows to compare contributions of the international community to Chornobyl-related research as well as integration of Ukraine in the international research on this subject. Furthermore, the content analysis of titles and abstracts of the publications allowed to detect the most important terms used for description of Chornobyl-related problems, see [I,95], [I,96], [II,42].

1.4.4 Algebraic graphs and their cryptographic applications:

In [I,109], [I,110], new multivariate cryptosystems were proposed over an n-dimensional free module over the arithmetical ring Zm based on the idea of hidden discrete logarithm for Zm*. These cryptosystems are based on the hidden Eulerian equations. If m is a “sufficiently large” product of at least two large primes, then the solution of the equation is hard without knowledge of the decomposition of m. In the Postquantum Era, one can solve the factorization problem for m and the discrete logarithm problem for Zm*. However, it does not lead to the straightforward break of such cryptosystem, because of the parameter α is unknown. Some examples of such cryptosystems were already proposed. We define their modifications and generalizations based on the idea of Eulerian transformations, which allow us to use asymmetric algorithms based on families of nonlinear multiplicatively injective maps with prescribed polynomial density and degree bounded by a constant.

Task 1.5: Describing kinetic and shape characteristics of micelle formation in branched polyethylene glycol containing amphiphiles on the increase of solute concentration. Comparison with available experimental data.

To describe kinetic and shape characteristics of micelle formation in branched amphiphiles, the mesoscopic simulation method of DPD has been employed. It describes polymer molecules on the level of coarse-grained beads each representing a fragment of the chain. The same applies to the water solvent, in which case a single solvent bead is assumed to contain several molecules of water. All beads representing both a polymer and water are spheres of the same diameter which provides the length-scale of the problem, whereas the energy scale is assumed to be equal to 1. The monomers are connected via harmonic springs, whereas the compressibility of a coarse-grained solvent at a number density of beads equal to 3 matches that for water at normal condition by a suitable choice for the parameter of the repulsive force acting between beads. Four types of molecular architectures are considered and all of them can be interpreted as four linear diblock copolymers, each of eight hydrophobic beads (type B) and of two hydrophilic beads (type A) bonded in a different way. In particular, architecture (a) is just a set of four non-bonded diblocks and serves as some kind of a reference system. Architecture (b) represents bonding of four diblocks in the form of an asymmetric miktoarm star of eight arms: four hydrophilic and four hydrophobic. The (c) and (d) architectures are of the diblock star type with the arms being bonded by either their hydrophobic ends, as in case (c), or by their hydrophilic ends, case (d). Molecular mass in all four cases is practically the same, save for an additional central bead in the cases (b)-(d), as compared to the case (a). First the aggregates have been identified and rejoined in space if split by the periodic boundary conditions. The analysis of their size and shape properties include the radius of gyration and the such shape characteristics as asphericity, prolateness and shape descriptor, all derived from the components of the gyration tensor of the aggregate, see [I,67].

Task 1.6: Studying the scaling properties for the micelle shape characteristics (radius of gyration and various universal combinations of gyration tensor components) obtained in Task 1.3 at the increase of molecular weight. Comparison with the corresponding scaling properties of polymer chains and polymer networks.

Scaling properties of the micelles shape characteristics were studied by simulating the aggregation of N_a star-like amphiphilic molecules immersed into water, see [I,64]. A single aggregate is observed as the result of equilibration and its shape characteristics are studied depending on the aggregation number N_a. The simulation study reveals strong dependencies of the shapes of aggregates formed by amphiphilic stars in water on the details of their molecular architecture. It has a prospect of the application in the drug delivery systems, where both the size and the shape of the aggregate is known to play an important role for the flow of the enveloped agent through the vessels. Four molecular architectures have been examined: (a) four disjoint linear diblocks, (b) asymmetric miktoarm polymer, (c) diblock star 1 (hydrophilic parts pointing outwards) and (c) diblock star 2 (hydrophilic parts next to a central bead). For all cases, the same general sequence of shapes is found with an increase of the aggregation number, namely: spherical micelle, aspherical micelle and a spherical vesicle. The "phase boundaries" between these are found to depend on the details of the molecular architecture. For the case (a)-(c), the transformation between a spherical and aspherical micelle occurs gradually, whereas the transition from an aspherical micelle into a spherical vesicle is in a form of a sharp transition. Histograms for the probability distributions of the shape descriptor are relatively narrow for both spherical micelle and spherical vesicle regimes but become wider next to the micelle-vesicle transition, indicating that a broad range of shapes are possible. The shape of the aggregate is found to oscillate between the rod-, disc-like and spherical with the period of oscillations strongly dependent on the molecular architecture. Both effects of slowing down and acceleration of these oscillations are found. These findings are relevant for the case of aggregates filled with water-insoluble drug agent, which will be a topic of the further studies.

Task 1.7: Constructing and studying Gibbs states of classical and quantum models (with `unbounded spins') on irregular and random graphs, also with random parameters, with special attention to phase transitions and the influence of the graph structure on the properties of Gibbs fields.

1.7.1 Revealing the universality class of the 2D Ising model with long-range correlated disorder:

In [I,27] and [I,28], we have studied critical behavior of the diluted 2D Ising model in the presence of disorder correlations which decay algebraically with distance as power law of *r* with decaying exponent a. Mapping the problem onto 2D Dirac fermions with correlated disorder we calculated the critical properties using the renormalization group perturbations up to two-loop order. We showed that besides the Gaussian fixed point the flow equations have non-trivial (i.e., non-Gaussian) fixed points.

1.7.2 Suggesting a new type of critical behavior in the Potts model with invisible states:

In [I,87] and [I,102], the mean-field Potts model with q interacting and r non-interacting (invisible) states had been reconsidered. The model was recently introduced to explain discrepancies between theoretical predictions and experimental observations of phase transitions in some systems where the Z_q-symmetry is spontaneously broken. We analyzed the marginal dimensions of the model, i.e., the value of r at which the order of the phase transition changes. In the q=2 case, we determined that value to be r_c =3.65(5); there is a second-order phase transition there when $r<r_c$ and a first-order one at $r>r_c$. We also analyzed the region $1 \leq q<2$ and show that the change from second to first order there is manifest through a new mechanism involving two marginal values of r. This new mechanism indicates how the discontinuity characteristic of first order phase transitions emerges. Also the exact solution of the 1D classical short-range Potts model with invisible states had been obtained, see [I,87]. We determined the partition function, using the transfer-matrix method, in the general case of two ordering fields. We analyzed the location of its zeros in the complex temperature plane.

1.7.3 Phase transitions in continuum classical systems with Curie-Weiss interactions:

Grand canonical equilibrium states of a continuum system of interacting particles are studied, see [I,79], [I,80], [I,81], [I,82], [I,83], [I,84], [II,37], [II,38], [II,39]. In the cell model studied in [I,79], [I,82], [I,83], [I,84], the particles are placed in the space $\boldsymbol{R}^d$ divided into congruent cubic cells. For a region V consisting of N cells, every two particles contained in V attract each other with intensity J/N. The particles contained in the same cell are subject to a binary repulsion with intensity $I > J$. For fixed values of the temperature, the interaction intensities and the chemical potential, the thermodynamic phase is defined as a probability measure on the space of occupation numbers of cells, determined by a condition typical to Curie-Weiss theories. There is proved that the half-plane $J\times$ chemical potential contains phase coexistence points at which two thermodynamic phases of the system exist. An equation of state for this system is obtained. A version of the continuum Widom–Rowlinson model is introduced and studied in [I,80] and [II,37]. It is a two-component gas of point particles placed in $\boldsymbol{R}^d$ in which like particles do not interact and unlike particles contained in a given vessel of volume V repel each other with intensity a/V. This model is thermodynamically equivalent to a one-component gas with multi-particle interaction. For both models, a rigorous theory of a phase transition is developed in the framework of the grand canonical formalism.

1.7.4 Gibbs states and phase transitions in continuum classical magnets:

Quenched thermodynamic states of an amorphous ferromagnet are studied in [I,21], [I,22], [I,23] [II,10]. The magnet is a countable collection of point particles chaotically distributed over $\boldsymbol{R}^d$, $d \geq 2$. Each particle bears a real-valued spin with symmetric a priori distribution; the spin-spin interaction is pair-wise and attractive. Two spins are supposed to interact if they are neighbors in the geometric graph defined by a homogeneous Poisson point process. For this model, we prove in [I,21], [I,23] that the following holds with probability one: (a) quenched thermodynamic states exist; (b) they are multiple if the particle density (i.e., the intensity of the underlying point process) and the inverse temperature are big enough; (c) there exist multiple quenched thermodynamic states which depend on the realizations of the underlying point process in a measurable way.

1.7.5 Gibbs states and phase transitions in quantum systems:

The basic elements of the mathematical theory of states of thermal equilibrium of infinite systems of quantum anharmonic oscillators (quantum crystals) are developed in [II,36]. 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. This effect can be established by analyzing the properties of the Matsubara functions corresponding to the global states. The equilibrium dynamics of finite subsystems can also be described by means of these functions. Then three basic results of this theory are presented and discussed: (a) a sufficient condition for a phase transition to occur at some temperature; (b) a sufficient condition for the suppression of phase transitions at all temperatures (quantum stabilization); (c) a statement showing how the phase transition can affect the local equilibrium dynamics. Two-time correlation functions of a system of Bose particles were studied in [I,50]. We found correlation of the zeros of the correlation functions with the Lee-Yang zeros of the partition function of the system. This gives the possibility to observe the Lee-Yang zeros experimentally. A particular case of a two-level system of Bose particles was examined and the zeros of the two-time correlation functions and the Lee-Yang zeros of the partition function of this system were analyzed. The two-time correlation function for a probe spin interacting with a spin system (bath) was examined in [II,23]. We showed that the zeros of this function correspond to the zeros of the partition function of a spin system in a complex magnetic field. The obtained relation gives a new possibility to observe the Lee-Yang zeros experimentally.

Task 1.8: Constructing and studying Gibbs states of quantum systems (lattice and continuous) with deformed commutation relations.

1.8.1 Correlation functions of a *q*-deformed Bose gas:

Time-dependent correlation functions of a *q*-deformed Bose gas were studied in [II,22]. We show how the zeros of the correlation functions are related to the Fisher zeros of the partition function of the system. The complex values of the temperature appear as the result of the q-deformation and the evolution of the correlation function. 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.

1.8.2 Algebras of noncommutative observables:

In [I,51], we constructed an algebra with non-commutative coordinates and momenta which is rotationally invariant and equivalent to a noncommutative algebra of canonical type. The influence of the non-commutativity on the energy levels of the hydrogen atom was studied in a rotationally invariant noncommutative phase space. We found corrections to the energy levels up to the second order in the parameters of non-commutativity and upper bounds for these parameters. It was shown that the coordinates in the noncommutative phase space depend on the mass; therefore, they cannot be considered as kinematic variables. Also, the noncommutative momenta are not proportional to the mass – as it is in the classical case. In [I,49], we found conditions on the parameters of noncommutativity under which these peculiarities can be incorporated into the theory. We also found that under the same conditions the weak equivalence principle is not violated, the properties of the kinetic energy are recovered, and the motion of the center of mass of the composite system and its relative motion are independent in the noncommutative phase. In [I,52], a two-particle system was studied for which the coordinates and the momenta do not commute. In this case, the non-commutativity parameters depend on the particle mass and this dependence can be different for each particle. The energy spectrum of the system was found for a particular type of the interaction. In [II,24], we studied a composite system in a noncommutative phase space with preserved rotational symmetry. We found conditions to the parameters of noncommutativity under which the commutation relations for the coordinates and momenta of the center of mass of the composite system reproduce the noncommutative algebra for the coordinates and momenta of the individual particles. Besides, it was shown that under these conditions the coordinates do not depend on the mass and can be considered as kinematic variables, the momenta are proportional to the mass. A two-particle system with Coulomb interaction was studied and the corrections to the energy levels of these system were found in the rotationally invariant noncommutative phase space. Thereby, the effect of noncommutativity on the spectrum of exotic atoms was analyzed. In [I,101], we reduced the two-body problem to the one-body problem in the general case of a deformed Heisenberg algebra leading to minimal length. Two-body problems with delta and Coulomb-like interactions were solved exactly. We obtained explicit expression for the energy spectrum for particular choices of the deformation function. The dependence of the energy spectrum on the center-of-mass momentum was found.

Deliverables:

D1.1: Joint research paper on equilibrium morphologies and percolation of nanoparticle-doped LCE in various mesophases: [I,61], [I,62] .

D1.2: Joint research paper on universal features of complex polymer and Gibbs states on regular and irregular structures: [I,65], [I,66], [II,30] (complex polymers), [I,85], [I,86], [II,35] (Gibbs states on irregular structures), [I,27], [I,87], [I,102] (Gibbs states on regular structures), [I,69], [I,95], [I,96], [II,42], [II,43] (other applications of irregular structures).

D1.3: Joint research paper on the micelle formation, shape characteristics: [I,66], [I,67], [II,30].

D1.4: Joint research paper on existence and properties of quantum and classical models on graphs and continuum particle configurations: [I,21], [I.22], [I,23], [I,79], [I,80], [I,81], [I,82], [I,83], [I,84], [II,10], [II,37], [II,38], [II,39] (classical models on continuum particle configurations), [I,28], [I,55], [I,87], [I,102] (other classical models), [I,50], [I,68], [II,23], [II,36] (quantum models).

D1.5: Joint research paper on quantum models with deformed commutation relations: [I,49], [I,51], [I,52], [I,101], [II,22], [II,24], [II,25].

Milestone 2: Structure of LCE and organic solar cells

Formation of a gel-like structure that mimics doped liquid crystal elastomer was studied by using computer simulations of a coarse-grained model of gold nanoparticles decorated by liquid crystalline ligands. First in the literature, photo-controllable gelation of this system was analyzed within a pore when the liquid crystalline groups are photosensitive azobenzene units [I,61], [I,62]. Experimentally observed repeated gel/dispersion cycles were reproduced by simulations and the wall-to-wall percolation was found to be essentially dependent on the concentration of nanoparticles. Wide spectrum of network properties such as: maximum subnetwork size and dimension, average vertex rank, local clustering coefficient and effective Hookean spring constant have been analyzed for LCE networks formed by patchy-decorated nanoparticles with various patching patterns [II,28]. It has been found that more symmetric patterns that produce gel with lower local clustering coefficient are more mechanically stable and more suitable for applications. The original focus planned for organic solar cells systems has been shifted towards applications in heterogeneous catalysis due to a large number of related synthetic and experimental studies of gold nanoparticles containing gels.

Work Package 2. Microscopic modeling in spatial and evolutionary biology.

Tasks 2.1 and 2.3: Elaborating and qualitative validating microscopic models of animal movement in random media.

The individual-based modeling of animal movement in random media – as a mathematical discipline – is at the very beginning of its development; thus, elaborating a standard set of general concepts, principles and tools is an actual task. Most of the mathematical methods available for nonlinear stochastic and spatial models are based on heuristic rather than mathematical assumptions, so that, e.g., the choice of the moment closure can be considered as an art rather than a science. In [I,97] we have made an essential step in solving this problem based on recent developments in specific branch of probability theory, Markov evolutions in the space of locally finite configurations. As a result, a general mathematically rigorous and practically useful framework has been elaborated that might be widely applicable in pursuing the mentioned tasks, as well as in other problems of theoretical ecology. In [II,9], we go further in this direction. By formulating a unified framework for a wide class of models of interest we develop methods that allow us to derive closed system of equations whose solutions give the next term of the approximation beyond the mean-field (mesoscopic) limit. The natural next step would be studying the space-time spreading of the solutions to these evolution equations. In [I,39], [I,40], [II,7], [II, 12], [II,14], we perform this study for the equations describing the spatial logistic model and its generalization towards including dispersion spreading and monostable reactions.

Tasks 2.2 and 2.4: Elaborating and qualitative validating microscopic models that connect individual behavior to population dynamics defined as Markov evolution in random media.

In pursuing these tasks, we mostly concentrated on studying models of infectious disease spread, for which we have obtained the following.

2.2.1 Analytic and computer simulation studying microscopic SIS models on graphs:

In the model elaborated, validated and studied in [I,58] and [I,60], each vertex of an underlying graph is occupied by an individual that can be in two states: susceptible or infected. The graph can be of the following two versions: (a) a regular one with vertex degree q; (b) the degree of each vertex is a globally bounded random variable (with bound Q), and the degrees of different vertices are independent. The vertex degree q is interpreted as the individuals' implicit (effective) mobility. These models are microscopic generalizations (that include also randomness of the environment) of the phenomenological (mean-field) SIS model, known in the literature. The individuals in these models undergo a (quenched) Markov-type evolution with discrete time run according to the asynchronous cellular automata algorithm. Such models can also be used to describe other communities of interacting biological species. The stationary states of the models were studied first, with the focus on the phase-transition-like behavior for the ratio of infected individuals J that vanishes at the critical curing rate γ^*. In case (a) (with fixed q), the critical curing rate γ^* increases towards its value 0.5 typical to the mean-field version, which in this case is obtained by taking $q=N$ (N being graph's order). For both versions, the results of simulations and the analytic study of the mean-field version were used to obtain an analytic interpretation of the stationary states. In particular, for different values of the curing rate γ the following three distinct behavior of the spatial patterning of infected individuals were found: (i) single cluster; (ii) large+small clusters; (iii) small clusters only. A phase-transition-like change between (ii) and (iii) is found to occur at $\gamma = \gamma^*$ -- the inflection point for the largest cluster size. The value of γ^* was found to be weakly dependent on q for the fixed q model. But it is remarkably dependent on the bound Q for the random graph version. It was found that the randomness promotes splitting of the largest cluster at lower q. In studying the dynamics of the models, we found that both the increase of q (in case (a)) and of its randomness (in case (b)) reduce the time needed by the system to reach the stationary state when the simulation is started from the almost healthy state. The type of the evolution of the spatial patterning also demonstrates strong dependence on the model type and the parameters of the run. For the contact-process-like infection spread with *q*=4, the grows of the number of the infected clusters towards its stationary value is always monotonic. With the increase of *q* beyond this value, the monotonicity disappears and the number of clusters shows a pronounced maximum about a mid-way towards its stationary value. This type of evolution -- which involves the initial built up of a huge number of separated clusters and their subsequent merge into larger ones -- is getting more pronounced for the model of type (b) (with random underlying graph).

2.2.2. Analytic and computer simulation studying microscopic SEIS models on graphs:

A more advanced version of the model mentioned in 2.2.1 is the SEIS model, in which each individual (attached to a vertex of the underlying graph) can be in the states: susceptible, exposed, infected, and then again susceptible. This model was introduced, validated and studied in [II,29] via the cellular automaton with the von Neumann neighborhood. The model is described by three parameters: encounter (contact) rate β, activation rate *p* and curing rate γ. The results, where possible, were compared to the ones obtained for the mean-field compartmental SEIS model. This allowed us to clarify the role of the local connectivity of individuals in the dynamics of the disease spread, its stationary states, as well as in the arrangement and spatial patterning of infected individuals. To study the spread dynamics the simulations were initiated from the state with fraction of infectious individuals equal 0.01 of the whole population. The growth of this fraction towards its stationary state value was observed in most of the cases. The critical curing rate γ* was defined as the curing rate at which both fractions of infectious I and exposed E individuals in the stationary state turn to zero. For γ > γ *, the characteristic time τ for the system to reach the stationary state increased rapidly indicating the critical slowing down effect. Assuming scaling behavior for τ the estimate for the dynamical critical exponent was made. The level of clustering in the system has been characterized by the number *K* of clusters of infectious individuals. In the stationary state, *K* as a function of γ attains maximum at a certain value γ < *K* on γ*, independent of *p* and β. To clarify the process of the cluster growth we performed additional simulations started from the state with a single infectious individual and visualizing the early-time single cluster development. At low curing rates γ, the cluster has approximately circular solid interior of infectious individuals with its external surface decorated by exposed individuals. Decoration density depends on the activation rate *p*. With the increase of γ, the interior is also getting decorated due to the development of cured individuals there and their subsequent exposure to the infection. Upon approaching γ*, the cluster structure appear to be fractal, but a more detailed analysis of its properties remains beyond the scope of this study.

Deliverables:

D2.1: Construction of the models of animal movement in random media, a joint research paper: [I,97], [II,9].

D2.2: Construction of models that connect individual behavior to population dynamics as Markov evolution models: [I,59], [I,60], [II,29].

D.2.3 Qualitative validation of the models of animal movement in random media, a joint research paper: [I,39], [I,40], [II,7], [II,14].

D2.4: Qualitative validation of the models that connect individual behavior to population dynamics as Markov evolution models: [I,59], [I,60], [II,29].

Milestone 3: Models of animal movement in random media

Achieved in deliverables D2.1 – D2.4.

Work Package 3. Microscopic (Markov) dynamics of continuum particle systems with applications.

Tasks 3.1 and 3.2: Studying microscopic Markov dynamics of spatial ecological models: identifying Markov generators and studying the corresponding dynamics.

3.1.1 Microscopic Markov dynamics of jump type.

In [II,6], we continue studying jump dynamics of an infinite system of particles in the continuum performing random jumps with repulsion – the case of free jumps was studied in [I,5]. As the states of the system we use probability measures on the space of infinite configurations of particles. Among them there are sub-Poissonian states defined as those the correlation functions of which are dominated by the correlation functions of Poissonian states. Such states are characterized by the lack of clustering. The main result of [II,6] is the construction of the global in time evolution of such states as weak solutions of the corresponding Fokker-Planck equations. In [I,78], a similar construction was carried out for an infinite system of particles performing random jumps with attraction of a certain kind. The main result of this work is the conclusion that, for a finite time horizon, the attraction of the considered kind is compatible with the sub-Poissonicity that corresponds to the absence of clustering in the system. In [I,6], we study a jump-dynamic model with two types of particles analogous in a sense to the Widom-Rowlinson model of phase transitions studied in [I,80] and [II,37]. Its birth-and-death version was introduced and studied in [I,38]. In the model introduced and studied in [II,6], the particles perform random jumps in $\boldsymbol{R^d}$ in the course of which particles of different types repel each other whereas those of the same type do not interact. The states of the system are probability measures on the corresponding marked configuration space. The global in time evolution of the states is constructed by means of correlation functions and generating functionals. It is proved that for each initial sub-Poissonian state μ_0, the states evolve in such a way that state μ_t is sub-Poissonian for all *t*>0. Possible phase transitions in this model were also discussed. In [I,98], there was studied an infinite system of point particles in $\boldsymbol{R^d}$ that perform random jumps with repulsion (as those in [II,6]) in the course of which two particles can coagulate. Similarly to the jumps the coagulations are subject to repulsion. The result of [I,98] is the solution of the kinetic equation describing this system.

3.1.2 Microscopic Markov dynamics of population models.

As adequate models describing collective behavior of large populations of interacting entities, we have identified infinite systems of particles in $\boldsymbol{R^d}$ with random birth (or immigration) and death (emigration) of the entities subject to competition or attraction. In [I,71], we studied a spatial ecological model in which the constituent entities reproduce themselves at distant points (disperse) and die with rate that includes a competition term. The system's states are probability measures on the space of configurations of entities, and their evolution is described by means of a hierarchical chain of equations for the corresponding correlation functions derived from the Fokker-Planck equation for the states. Under the conditions imposed on the model parameters identified in the paper, it was proved that the correlation functions evolve in a scale of Banach spaces in such a way that each correlation function corresponds to a unique sub-Poissonian state. In [I,75] and [II,33], we continue studying such systems where we focus on the effect of self-regulation in the population. Namely, we demonstrate the role of the tradeoff between the dispersal and competition in such systems. In [I,76], we study the Markov evolution of states of a continuum migration model. It describes an infinite system of entities placed in $\boldsymbol{R^d}$ in which the constituents appear (immigrate) with state dependent rate and disappear (emigrate), also due to competition. For this model, we prove the existence of the evolution of states such that the moments of the number of entities in compact subsets of $\boldsymbol{R^d}$ remain bounded for all *t*>0 due to the competition between the entities. Under an additional condition identified in this work, we prove that the density of entities and the second correlation function remain bounded globally in time. A number of properties of a special kind of population models – so called spatial logistic models – were studied in [II,27]. A model of an infinite population with fragmentation was proposed and studied in [I,107]. In this model, the point entities undergo fission (splitting) into a finite random number of new entities. Such processes can model e.g., division of biological cells. The main result of [I,107] is the description of the evolution of correlation functions in a scale of Banach spaces. In [I,64], the dynamics of an infinite structured population of entities with age was introduced and studied. The main aspect of this dynamics is aging – drifting in the direction of increasing age. For this system, the evolution of the correlation functions of first and second order was described. A model describing the propagation of particles as a nonlocal diffusion was proposed and studied in [II,12].

3.1.3 General theory configuration spaces and related stochastic processes.

In [II,45], a general approach to studying the statistical mechanical properties of interacting particle systems was developed that employs considering the system at different hierarchical levels. In [II,16], general methods were developed to study non-linear perturbations of particle systems evolving in scales of Banach spaces. In [I,2] and [II,40], we studied measure preserving mappings between probability spaces and identified conditions under which the mapping preserves the discreteness and the relations “to be singular” and “to be absolutely continuous” between the measures on the initial space and the corresponding image measures. For several important families of probability measures (including multidimensional cases), these results were applied to solve the corresponding problems of the Markov dynamics on configuration spaces. We also studied properties of random variables with independent GLS-symbols. Conditions for fine covering families of GLS-cylinders to be faithful for the calculation of the Hausdorff dimension were identified. By means of these results we studied fine fractal properties of singularly continuous measures with i.i.d. GLS-symbols. A number of them were generalized to the general ML-case. We also developed a probability approach to the study of fine fractal properties of subsets of non-normal numbers w.r.t. GLS-expansions. We proved, in particular, that the set of GLS-essentially non-normal numbers is of full Hausdorff dimension. We have shown that this set is of the second Baire category for any GLS-expansion. In [I,3] and [II,19], we developed the dimension preserving approach to the study of fractal properties of subsets of I-Q∞-non-normal numbers and prove that the set of I-Q_∞-quasinormal numbers, the set of I-Q_∞-partially non-normal numbers and the set of I-Q_∞-essentially non-normal numbers are of full Hausdorff dimension. It was also shown that the set of I-Q∞-essentially non-normal numbers is a comeager set, and, therefore all other above mentioned subsets are of the first Baire category. In [II,31] and [II,32], we developed the basis of the analysis on configuration spaces and *p*-adic spatial combinatorics. Analysis on configuration spaces is a kind of infinite-dimensional analysis closely connected with several branches of mathematics including representation theory, theory of point processes and especially with mathematical physics, in particular statistical mechanics of infinite systems of interacting particles. We defined and studied non-Archimedean versions of the main notions of analysis on configuration spaces including the construction of a K-transform and the infinite-dimensional umbral calculus. In [I,70] and [II,5], we consider a nonlinear evolution equation for complex-valued functions of a real positive time variable and a *p*-adic spatial variable. This equation is a non-Archimedean counterpart of the fractional porous medium equation. Developing, as a tool, an *L*1-theory of Vladimirov’s *p*-adic fractional differentiation operator, we prove *m*-accretivity of the appropriate nonlinear operator, thus obtaining the existence and uniqueness of a mild solution. In [I,30] and [II,16], the study of semigroups of composition operators and semigroups of holomorphic mappings was performed. We establish conditions under which these semigroups can be extended in their parameter to a sector given a priori. We show that the size of this sector can be controlled by the image properties of the infinitesimal generator, or, equivalently, by the geometry of the so-called associated planar domain.

Tasks 3.3 and 3.4 Deriving a priori information on the behavior of the processes, including those with random parameters. Studying ergodic properties of these processes (existence of invariant or stationary states).

Some general aspects of the ergodic theory in applications to the systems of interest were studied in [I,89]. The *p*-adic theory of the motion in porous random medium was studied in [II,5]. In [II,2] and [II,4], we studied properties of Bernoulli convolutions generated by the second Ostrogradsky series and proved that the corresponding measure has the spectrum of the zero Hausdorff dimension and its Fourier-Stieltjes transform does not tend to zero at infinity. We developed different approaches to estimating a level of "irregularity" of probability distributions whose spectra are of zero Hausdorff dimension. Using generalizations of the Hausdorff measures and dimensions, fine fractal properties of the above probability measures are studied in details. Conditions for the Hausdorff-Billingsley dimension preservation on the spectrum by its probability distribution function were also obtained. In [I,47], [I,56], [I,57] and [I, 106], we developed probabilistic and metric theory of abstract F-expansions of real number, which include as partial cases the well-known Sylvester expansion, second Ostrogradskiy expansion, Q*-expansion, Ostrogradskiy-Sierpinski-Pierce expansion, Engel expansion for real numbers. Conditions under which for almost all (w.r.t. Lebesgue measure) real numbers from the unit interval their F-expansion contains arbitrary digit i only finitely many times are found. Based on results on metric theory of F-expansion we developed a unified approach for proving singularity (w.r.t. Lebesgue measure) of distributions of random variables independent symbols of Sylvester, second Ostrogradskiy, Ostrogradskiy-Sierpienski-Pierce and Engel expansions. In [II,3] and [II, 34], we studied properties of subsets of non-normal numbers w.r.t. Cantor series expansion for a class of bases of full measure for shift invariant ergodic probability measures on {2, 3, …} N satisfying a mild condition. We improved the previous results by showing that essentially non-normal numbers have full Hausdorff dimension considering numbers not only whose digital frequencies do not exist but whose block frequencies also do not exist. Also, we shown that this set is of second Baire category. In [II,15], we developed umbral calculus on the space *D′* of distributions on $\boldsymbol{R}^d$, which leads to a general theory of Sheffer sequences on *D′*. We defined a sequence of monic polynomials on *D′*, a polynomial sequence of binomial type, and a Sheffer sequence. We presented equivalent conditions for a sequence of monic polynomials on *D′* to be of binomial type or a Sheffer sequence, respectively. Our theory has remarkable similarities to the classical setting of polynomials on ***R***. The form of the generating function of a Sheffer sequence on *D′* is similar to the generating function of a Sheffer sequence on ***R***, albeit the constants appearing in the latter function are replaced in the former function by appropriate linear continuous operators. We constructed a lifting of a sequence of monic polynomials on ***R*** of binomial type to a polynomial sequence of binomial type on *D′*, and a lifting of a Sheffer sequence on R to a Sheffer sequence on *D′*. Examples of lifted polynomial sequences include the falling and rising factorials on *D′*, Abel, Hermite, Charlier, and Laguerre polynomials on *D′*. Some of these polynomials have already appeared in different branches of infinite dimensional analysis and played there a fundamental role.

Task 3.5 Studying holomorphic generating functionals.

The evolution of states of continuum infinite particle systems constructed in [I,6], [I,71], [I,76] and [II,6] was constructed, in fact, by solving the corresponding evolution equation for the generating (so called Bogoliubov) functionals. The main problem of this construction is the identification of the evolving functionals and generating functionals of probability measures. That is, starting from a Bogoliubov functional B_0 we obtain B_t as the solution of the corresponding evolution equation. Thereafter, we have to prove that this solution is the generating functional corresponding to a certain state μ_t. To do this, we developed a technique based on some advanced methods of functional analysis, e.g., on the theory of $C_0 -$ semigroups and on the Denjoy-Carleman theorem. Generating functionals of measures studied in [I,6], [I,71], [I,76] and [II,6] can be extended to holomorphic maps of infinite-dimensional Banach spaces. Thus, their study is closely related to the study of a number of general properties of such maps. In [I,13], [I,14], [I,15] , [I,16] a tedious study of the iterates of holomorphic mappings in complex Banach spaces was conducted. Some of them, including boundary properties, were further studied in [I,7], [I,9], [I,31], [I,41] and [II,11]. A more general case of holomorphic mappings in J*-algebras was studied in [I,29]. Topological properties of the corresponding complex Banach spaces of a certain kind (used in the study of the generating functionals) were considered in [I,17], [I,18].

Deliverables:

D3.1 Joint research papers on constructing the dynamics for Markov generators with birth-and-death and jump parts: [I,5], [I,34], [I,35], [I,71], [I,75], [I,76], [I,77], [II,6], [II,27], [II,33].

D3.2 Joint research papers on constructing the Markov dynamics of multi-type systems: [I,6], [I,38].

D3.3 Joint research papers on constructing the dynamics of system of entities with continuous marks: [I, 64], [II,12].

D3.4 Joint research papers on constructing the dynamics which includes coagulation and fragmentation: [I,36], [I,98], [I,107].

D3.5 Joint research papers on constructing the dynamics with random parameters and/or in random environment: [I,70], [II,5].

D3.6 Joint research papers on studying the ergodic and similar properties of the processes as in D3.1 – D3.4: [I,1], [I,4], [I,88], [I,89], [I,103], [I,104], [II,2], [II,4].

D3.7 Joint research papers on studying the evolution of generating and holomorphic functionals of models as in D3.1 – D3.4: [I,6], [I,7], [I,8], [I,33], [I,42], [I,54], [I,71], [I,76], [II,6].

Milestone 4: Microscopic Markov and time-delay dynamic

Achieved in deliverables D3.1 – D3.7.

Work Package 4. Meso- and macroscopic dynamics of continuum particle systems with applications.

Tasks 4.1 and 4.2 Developing and applying different types of mesoscopic scaling of microscopic Markov evolutions.

The mesoscopic level of description of an infinite particle system is obtained by a scaling procedure. In [I,34], [I,35] and [I,38] Vlasov- and Kac-type scaling procedures were applied to obtain the mesoscopic (kinetic) equations describing birth-and-death and jump models. In [I,6], we have developed a scaling procedure which combines features of both Kac- and Vlasov-type scaling techniques. The main idea is to use the fact that the homogeneous Poisson state (corresponding to the lack of interactions) is scale-invariant in both mentioned techniques. Then a state is said to be Poisson-approximable if there exists a scaling procedure by which this state can be transformed into a Poisson state. Then the main aspect of the theory is to study whether such approximability is preserved in the course of the evolution in question. In [I,72], by means of general convolutional derivatives the related fractional statistical dynamics of continuous interacting particle systems was studied. We apply the subordination principle to construct kinetic fractional statistical dynamics in the continuum in terms of solutions to Vlasov-type hierarchies. Conditions for the intermittency property of fractional kinetic dynamics are obtained. In [I,27], the scaling behavior of model C was studied. The model describes the dynamics of an *n*-component non-conserved order parameter coupled statically to a scalar conserved density in an *d*-dimensional space. Conditions for the realization of different types of scaling regimes in the (*n,d*) - plane were studied within the field-theoretical renormalization group approach. Borders separating these regions were calculated on the base of high-order RG functions using ϵ-expansions as well as by fixed dimension *d* approach with re-summation. Also the critical properties of the three-dimensional Ising model with linear parallel extended defects were analyzed. Such a form of disorder produces two distinct correlation lengths. Estimates of quantitative characteristics of the critical behavior for such systems were only obtained up to now within the renormalization group approach. We report a study of the anisotropic scaling in this system via Monte Carlo simulation of the three-dimensional system with Ising spins and non-magnetic impurities arranged into randomly distributed parallel lines. Several independent estimates for the anisotropy exponent of the system had been obtained, as well as an estimate of the susceptibility exponent.

Task 4.3 Elaborating hydrodynamic scaling techniques leading from micro- to the macroscopic level.

In [I,90], a unified approach is proposed to describe the statistics of the short-time dynamics of multiscale complex systems. The probability density function 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. The dynamics of the background is formulated as a hierarchical stochastic model whose form is derived from simple physical constraints, which in turn restrict the dynamics to only two possible classes. The probability distributions of both the signal and the background have simple representations in terms of Meijer G functions. The two universality classes for the background dynamics manifest themselves in the signal distribution as two types of tails: power law and stretched exponential, respectively. A detailed analysis of empirical data from classical turbulence and financial markets shows excellent agreement with the theory. The hydrodynamic behavior of particle systems was studied in [I,111] and [I,112]. One of the most important problems is to describe the dynamics of a fluid in an irregular environment. In [I,112], there was studied the problem of vortex flows past a cylinder near a wall through the lenses of the point-vortex model. By conformally mapping the fluid domain onto an annular region in an auxiliary complex plane, we compute the vortex Hamiltonian analytically in terms of certain special functions related to elliptic theta functions. A detailed analysis of the equilibria of the model is then presented. The location of the equilibrium in front of the cylinder is shown to be in qualitative agreement with recent experimental findings. It was also shown that a topological transition occurs in phase space as the parameters of the systems are varied. In [I,111], analytical solutions for both a finite assembly and a periodic array of bubbles steadily moving in a Hele-Shaw channel are presented. The particular case of multiple fingers penetrating into the channel and moving jointly with an assembly of bubbles is also analyzed. The solutions are given by a conformal mapping from a multiply connected circular domain in an auxiliary complex plane to the fluid region exterior to the bubbles. In all cases the desired mapping is written explicitly in terms of certain special transcendental functions, known as the secondary Schottky-Klein prime functions. These solutions for a complete set of solutions for steady bubbles and fingers in a horizontal Hele-Shaw channel when surface tension is neglected. All previous solutions under these assumptions are particular cases of the general solutions obtained in [I,111]. A *p*-adic version of the theory of the motion in porous media was studied in [I,70].

Task 4.4 Studying front propagation, invasion, homogenization, pattern formation and their long-time asymptotic.

In [I,74], there was studied a ground state of some non-local Schrödinger operator associated with an evolution equation for the density of population in the stochastic contact model in the continuum with inhomogeneous mortality rates. A new effect in this model was found when even in the high-dimensional case a small positive perturbation of a special form (so-called, small paradise) implies the appearance of the ground state. In [I,73], there were studied spectral properties of a convolution operators L and their perturbations in the form $H=L+v(x)$ by compactly supported potentials. The results obtained are applied to describe the front propagation of a population density governed by the operator H with a compactly supported initial density provided that H has positive eigenvalues. If there is no positive spectrum, then the stabilization of the population density is proved. In [I,36], there was studied the stability of stationary solutions for a class of nonlocal semi- linear parabolic equations. To this end, we proved the validity of the Feynman–Kac formula for a Lévy processes with time-dependent potentials and arbitrary initial condition. Then we found sufficient conditions for the asymptotic stability of the zero solution to hold, and used them to the study of the spatial logistic equation arising in population ecology. For this equation, we found conditions which imply that its positive stationary solution is asymptotically stable. We considered also the case where the initial condition is given by a random field. In [I,40], we considered the accelerated propagation of solutions to equations with a nonlocal linear dispersion on the real line and monostable nonlinearities (both local or nonlocal, however, not degenerated at 0), in the case where either of the dispersion kernel or the initial condition has regularly heavy tails at both $\pm\infty$, possibly different. We showed that, in such a case, the propagation to the right is fully determined by the right tails of either the kernel or the initial condition. We described both cases of integrable and monotone initial conditions which may give different orders of the acceleration. Our approach was based, in particular, on the extension of the theory of sub-exponential distributions introduced here and studied in [II,13]. In the latter work, we showed that the n-fold convolution of a sub-exponential probability density on the real line is asymptotically equivalent to this density times n. We proved Kesten's bound, which gives a uniform in n estimate of the n-fold convolution by the tail of the density. We also introduced a class of regular sub-exponential functions and use it to find an analogue of Kesten's bound for functions on $\boldsymbol{R^d}$. The results were applied for the study of the fundamental solution to a nonlocal heat equation. In [II,12], we described the acceleration of the pulled front propagation for the solutions to a class of monostable nonlinear equations with a nonlocal diffusion in $\boldsymbol{R^d}$. We showed that the acceleration takes place if either the diffusion kernel or the initial condition has 'regular' heavy tails in $\boldsymbol{R^d}$ (in particular, decays slower than exponentially). Under general assumptions which can be verified for particular models, we presented sharp estimates for the time-space zone which separates the region of convergence to the unstable zero solution with the region of convergence to the stable positive constant solution. We showed the variety of different possible rates of the propagation starting from a little bit faster than a linear one up to the exponential rate. We described differences between the case when the initial condition decays in all directions at infinity with the case of the initial condition decreasing along all coordinate axes (in positive directions). Turbulence is a challenging feature common to a wide range of complex phenomena. Random fiber lasers are a special class of lasers in which the feedback arises from multiple scattering in a one-dimensional disordered cavity-less medium. In [I,100], we studied statistical signatures of turbulence in the distribution of intensity fluctuations in a continuous-wave-pumped erbium-based random fiber laser, with random Bragg grating scatterers. The distribution of intensity fluctuations in an extensive data set exhibits three qualitatively distinct behaviors: a Gaussian regime below threshold, a mixture of two distributions with exponentially decaying tails near the threshold and a mixture of distributions with stretched-exponential tails above threshold. All distributions are well described by a hierarchical stochastic model that incorporates Kolmogorov's theory of turbulence, which includes energy cascade and the intermittence phenomenon.

Deliverables:

D4.1 Joint research papers on the Vlasov-type scaling procedure and controlling the convergence in the scaling limit: [I,34], [I,35], [I,36].

D4.2 Joint research papers on the Kac-type scaling procedure and controlling the convergence in the scaling limit: [I,6].

D4.3 Joint research papers on the moderate scaling procedure for potential and controlling the convergence in scaling limit:[I,72].

D4.4 Joint research papers on multi-scaling procedures in various, complex microscopic dynamics: [I,90], [I,100], [II,13].

D4.5 Joint research papers on the moderate scaling limit for a number of dynamics: [II,14]

D4.6 Joint research papers on nonlinear and nonlocal equations with special attention to such phenomena as pattern formation, front propagation, long-time asymptotic: [I,40], [I,73], [I,74], [I,100], [II,12].

D4.7 Joint research papers on nonlinear and nonlocal equations with random environment and/or random interactions: [I,38], [I,70], [I,71], [II,13].

Milestone 5: Scaling techniques for meso- and macro descriptions.

Achieved in deliverables D4.1 – D4.7.

Work Package 5. Compartmental models with time delays and stochasticity.

Tasks 5.1 and 5.2 Elaborating principles for the formulation of linear and nonlinear compartmental models with general (non-Markovian) residence time distributions and mathematical techniques for their studying.

Individual-based models – IBMs – naturally describe the dynamics of interacting organisms or social (e.g., financial) agents. They are considered too complex for mathematical analysis, but computer simulations of them cannot give the general insights required. In [II,9] we propose a resolution of this problem by constructing a general mathematical framework for IBMs containing interactions of an unlimited level of complexity, and derive equations that reliably approximate the effects of space and stochasticity. We provided software, specified in an accessible and intuitive graphical way, so any researcher can obtain analytical and simulation results for any particular IBM without algebraic manipulation. We illustrated the framework with examples from movement ecology, conservation biology, and evolutionary ecology. This framework will provide unprecedented insights into a hitherto intractable panoply of complex models across many scientific fields. In [I,99] and [I,105], a similar theory was developed that can be applied to analyzing complex behavior of option markets. In [I,46], we have elaborated a new approach to studying compartmental models based on the Ricker model – one of the most widely-used ecological models displaying complex nonlinear dynamics. We study a discrete-time population model, which is derived from simple assumptions concerning individual organisms' behavior. In the large-population limit the model converges to the Ricker model, and can thus be considered a mechanistic version of the Ricker model, derived from basic ecological principles, and taking into account the demographic stochasticity inherent to finite populations. We employ several analytical and precise numerical methods to study the model, showing how each approach contributes to understanding the model's dynamics. Expressing the model as a Markov chain, we employ the concept of quasi-stationary distributions, which are computed numerically, and used to examine the interaction between complex deterministic dynamics and demographic stochasticity, as well as to calculate mean times to extinction. A Gaussian Markov chain approximation is used to obtain quantitative asymptotic approximations for the size of fluctuations of the stochastic model's time series around the deterministic trajectory, and for the correlations between successive fluctuations. The results are compared to those obtained from quasi-stationary distributions and simulations.

Task 5.3 Revisiting **c**lassical and recent models of mathematical biology with the aim of developing more realistic versions of such models by incorporating non-exponential residence-time distributions.

5.3.1. Stationary states of the SICS models of the disease with competing ordinary and drug-resistant carriers:

In [I,59], a simple SICS epidemiology model has been elaborated to describe principal features of the disease evolution with ordinary and drug-resistant carriers. It is suitable for both analytic and computer simulation studies. Along with the compartments of susceptible and infected individuals (as in an SIS model), this model includes also the compartment (C) of the individuals infected with the drug-resistant strain. The infecting and curing rates β and γ, respectively, are model parameters. The model also includes the transitions rules S → C, C → S and I → C. For simplicity, it is assumed that the infecting rate does not depend on the strain type, and thus the same infecting rate β is assigned to both S → I and S → C events. The unidirectional conversion I → C takes place with rate δ, whereas no reverse conversion is possible. Finally, the individuals from C compartment are cured with rate γ' which is different from that from I compartment, γ. This mimics the real therapeutic situation when the patient infected with a drug-resistant strain is cured by the second- or third-line antibiotics with different curing effectiveness. The stationary state of the SICS model were found. It was shown that in order to reduce the population of the most dangerous – resistant – strain, one should either minimize the conversion rate δ, or – if the latter is problematic – to increase the curing rate γ and decrease the infecting rate β. Despite the fact that such a result is qualitatively obvious, the explicit form of the stationary state solutions provides useful information for the quantitative evaluation of the effects related to each of these rates. These provide a good starting point for the further investigation of this SICS model for the disease with both ordinary and resistant carriers, and for its future generalization targeted on particular diseases (e.g. tuberculosis). In particular, one may extend this study to the analysis of stability of its solutions, to considering the case with unequal infecting rate for the ordinary and resistant carriers, as well as to the dynamics and spatial patterning of individuals.

5.3.2. Modeling epidemics by using multiple datasets.

Massive datasets obtained recently during pandemic spread of some viral diseases create the opportunity to revisit classical compartmental models with the aim to fit them for investigating the pandemic dynamics. In the case of A/H1N1 influenza, this was realized in [I,113] where a conditional likelihood approach was employed for fitting a disease transmission model to virological and serological data, conditional on clinical data. The model is used to reconstruct the temporal pattern of the pandemic in Israel in five age-groups and evaluate the factors that shaped it. We estimate the reproductive number at the beginning of the pandemic to be R = 1.4. We find that the combined effect of varying absolute humidity conditions and school vacations (SVs) is responsible for the infection pattern, characterized by three epidemic waves. Overall attack rate is estimated at 32%

(28–35%) with a large variation among the age-groups: the highest attack rates within school children and the lowest within the elderly. This pattern of infection is explained by a combination of the age-group contact structure and increasing immunity with age. We assess that SVs increased the overall attack rates by prolonging the pandemic into the winter. Vaccinating school children would have been the optimal strategy for minimizing infection rates in all age-groups. A similar study of the spread of polio was performed in [I,114].

Deliverables:

D5.1 Joint research papers on the methodology of construction of compartmental models with non-exponentially distributed residence times: [II,9], [I,46], [I,99], [I,105].

D5.2 Joint research papers on the mathematical analysis of such models and the necessity of extending classical tools and developing new tools: [I,59].

D5.3 Joint research papers on the applications of models of the above type to the modeling of biological phenomena: [I,113], [I,10].

Work Package 6. Mathematics and physics of the evolution of complex shapes.

Task 6.1 Elaboration and refinement of the Gaussian Free Field (GFF) approach to non-perturbative minimal models of the field theory.

We use the general Löwner theory to define general slit Löwner chains in the unit disk, which in the stochastic case lead to slit holomorphic stochastic flows, see [II,46]. Radial, chordal and dipolar SLE are classical examples of such flows. Our approach, however, allows constructing new processes of SLE type that possess conformal invariance and the domain Markov property. The local behavior of these processes is similar to that of classical SLEs [I, 19], [I,20], [I,95], [I,96].

Task 6.2 Construction of a homotopy of an arbitrary shape to a given canonical one by means of deterministic Löwner and Löwner-Kufarev evolutions

The Löwner equation is known as a one-dimensional reduction of the Benney chain as well as the dispersionless KP hierarchy. We propose a reverse process showing that time splitting in the Löwner or the Löwner-Kufarev equation leads to some known integrable systems. We study an embedding of the Loewner-Kufarev trajectories into the Segal-Wilson infinite dimensional Grassmannian, construct the tau-function, and the Baker-Akhiezer function which are related to a class of solutions to the KP hierarchy, see [I, 101], [I,106], [I,107]. The space of shapes was studied, applying the methods of the conformal evolution, deforming the unit circle. In [II, 47], we gave a Hamiltonian formulation of this evolution and provided conservation laws basing on the Löwner-Kufarev equation.

Task 6.3 Construction of families of stochastic counterparts to the Löwner and Löwner-Kufarev evolutions.

The Bogomol'nyi – Prasad – Sommerfeld (BPS) problem of wall crossing has attracted much attention the last ten years. Considering 4-dimensional theories coupled to surface defects, particularly the theories of class S, Gaiotto, Moore, and Neitzke introduced spectral networks of the trajectories on Riemann surfaces obeying certain local rules aiming at the characterization of possible spectra of BPS states and their changes under continuous deformations. Given a compact Riemann surface R with punctures and a Lie algebra of ADE type, e.g., SU(2) in our case, there exists a corresponding four-dimensional quantum field theory. The spectral network is defined by the critical trajectories of a quadratic differential which defines a singular measures foliation on R with singularities at the zeros and poles of q, see [I,43]. We described a graph parametrization of rational quadratic differentials with presence of a simple pole which critical trajectories form a network depending on parameters and focusing on the network topological jumps, see [I,41].

Task 6.4 Coupling GFF and the stochastic shape evolution.

We consider a coupling of the Gaussian free field with slit holomorphic stochastic flows, called (δ, σ)-SLE, which contains known SLE processes (chordal, radial, and dipolar) as particular cases. In physical terms, we study a free boundary conformal field theory with one scalar bosonic field, where Green's function is assumed to have some general regular harmonic part. We establish which of these models allow for coupling with (δ, σ)-SLE, or equivalently, when the correlation functions induce local (δ, σ)-SLE martingales (martingale observables), see [I, 63] and [I, 108].

Task 6.5 Construction of observables for the shape evolution and implementation of the singular representations of the chiral algebras.

It was realized recently that the chordal, radial and dipolar SLEs are special cases of a general slit holomorphic stochastic flow. We characterize those slit holomorphic stochastic flows, which generate level lines of the Gaussian free field. In particular, we describe the modifications of the Gaussian free field (GFF) corresponding to the chordal and dipolar SLE with drifts. Finally, we develop 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, see [I, 63].

Task 6.6 Relation of different interface evolutions and exactly solvable models.

In [I, 111] and [II, 41], 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. The probability distribution of velocity increments is calculated explicitly and expressed in terms of generalized hypergeometric functions of the type nF0, which exhibit power-law tails. The model predictions are found to be in good agreement with experiments on a low temperature gaseous helium jet. It is argued that distributions based on the functions nF0 might be relevant also for other physical systems with multiscale dynamics.

Task 6.7 Computer simulation of evolutions of random and deterministic interfaces.

In [II,44], we developed new methods of numerical solution of the general Löwner chains and simulation of the forward the general SLE. A general method for the approximation of conformal maps was introduced D.Marshal and S.Rohde in 2017. Numerical simulation of the general SLE was developed by the team of the project and implemented independently by using Wolfram Mathematica software. We described the applied method together with some technical difficulties, which motivates the structure of the program. The correctness (convergence) in the deterministic case was proved earlier by D.Marshal and S.Rohde. The analogous statement for the stochastic case is more difficult.

Deliverables:

D6.1 Joint papers on the obtained results related to the tasks of the work package: [I,20], [I,43], [I,100], [I,105], [I,108].

D6.2 Protocol for computer simulation of random and deterministic contour evolutions: [II,44].

D6.3 Web-site of the network:
http://folk.uib.no/ima083/strevcoms.html

D6.4 Report on the workshops will appear on the web-site:
http://folk.uib.no/ava004/Voss2016/index.html

Milestone 6: Evolution of complex shapes

Achieved in deliverables D6.1 – D6.4.

Work Package 7. Geometry of the space of shapes and pattern recognition.

Task 7.1 Definition of the space of shapes as an infinite-dimensional manifold of smooth curves.

In [I,91] and [I,93], we studied an embedding of the Löwner-Kufarev trajectories into the Segal-Wilson infinite dimensional Grassmannian, constructed the tau-function, and the Baker-Akhiezer function which are related to a class of solutions to the KP hierarchy. The space of shapes was studied, applying the methods of the conformal evolution, deforming the unit circle. We gave a Hamiltonian formulation of this evolution and provided conservation laws based on the Löwner-Kufarev equations. The conservative moments of the evolution were given by the Virasoro algebra, where the positive Virasoro generators span the holomorphic part of the complexified vector bundle over the space of conformal embeddings of the unit disk into the complex plane. The negative Virasoro generators can be recovered by an iterative method making use of the canonical Poisson structure, see [I,92].

Task 7.2 Comparison of metrics on the space of shapes and determination of shape statistics.

In [I,10] and [I,11], we study Fuglede's p-module of systems of measures in condensers in Euclidean spaces and on polarizable Carnot groups. We apply and generalize a result by Rodin, which provides an explicit method for finding the extremal function and the 2-module of a foliated family of curves in R2, to a variety of settings. In the planar case, we apply Rodin's method to obtain estimates for the conformal module of a parallelogram and of a ring domain using directional dilatations. In the Euclidean space, we identify the extremal function and compute the p-module of images of families of connecting curves and of separating sets with respect to the plates of a condenser under homeomorphisms of certain regularity. Then we calculate the module and find the extremal measures for the spherical ring domain on polarizable Carnot groups and extend Rodin's theorem to the spherical ring domain on the Heisenberg group.

Task 7.3 Probabilistic models of shapes, construction of probabilistic measures

In [I,41] and [I,42], 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.

Task 7.4 Elaboration of sub-Riemannian geometry and geometric control with constrains on infinite-dimensional manifolds with special attention to Lie groups.

By considering Riemannian submersions, in [II,26] we find necessary and sufficient conditions for the situation when sub-Riemannian normal geodesics project to curves of constant first geodesic curvature or constant first and vanishing second geodesic curvatures. We describe a canonical extension of the sub-Riemannian metric and study geometric properties of the obtained Riemannian manifold.

Task 7.5 Controllability in the space of shapes, shape tuning.

In [II,17], we study possible cases of complex simple graded Lie algebras of depth 2, which are the Tanaka prolongations of pseudo H-type Lie algebras arising through representation of Clifford algebras. We show that the complex simple Lie algebras of type B_n with |2|-grading do not contain non-Heisenberg pseudo H-type Lie algebras as their negative nilpotent part, while the complex simple Lie algebras of types A_n, C_n and D_n provide such a possibility. Among exceptional algebras only F_4 and E_6 contain non-Heisenberg pseudo H-type Lie algebras as their negative part of |2|-grading. An analogous question addressed to real simple graded Lie algebras is more difficult, and we give results revealing the main differences with the complex situation, see [I,53].

Task 7.6 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 is realized in [II,1]. We show that a 2-step nilpotent Lie algebra is isomorphic to its standard pseudo-metric form, that is a 2-step nilpotent Lie algebra endowed with some standard non-degenerate scalar product compatible with the Lie bracket, see [I,44] This choice of the standard pseudo-metric form allows us to study the isomorphism properties. If the elements of the centre of the standard pseudo-metric form constitute a Lie triple system of the pseudo-orthogonal Lie algebra, then the original 2-step nilpotent Lie algebra admits integer structure constants. Among particular applications we prove that pseudo H-type algebras have bases with rational structure constants, which implies that the corresponding pseudo H-type Lie groups admit lattices, see [I,44], [I,45], [II,18], [II,20]. Moreover the complete classification of pseudo H-type Lie algebras is finished.

Task 7.7 Elaboration of computationally feasible algorithmic and statistical procedures to perform computer simulation of shapes.

In [II,44], we considered a method of numerical simulation for (δ,σ)-Löwner chains. The problem becomes more complicated when the driving function is a sample of a random process such as the Brownian motion. This is due to the fact that we have to sample the process during the simulation. We prefer to avoid sampling of Brownian motion beforehand, because we do not know the partition in advance, because the required amount of floating-point operations and memory is incredibly big if we just take the smallest possible mesh and sample the Brownian motion uniformly in all points.

Deliverables:

D7.1 Joint papers on the obtained results related to the tasks of the work package: [I,10], [I,11], [I,41], [I,44], [I,45], [II,17], [II,18], [II,20],[II,26].

D7.2 Report on the workshop will appear on the web-site:

http://folk.uib.no/ava004/Voss2016/index.html

D7.3 Protocol for pattern recognition and shape analysis: [II,44].

Milestone 7: Complex shapes and computer vision

Achieved in deliverables D7.1 – D7.3.