C. **Research project description** *(maximum 10 pages and maximum 2 pages bibliography)*

D1. Issues

The classical methods and models of statistical physics proved to be useful for understanding the large variety of spatial and/or temporal structures that are present in physical and socio-economic phenomena. Most of the intriguing patterns arise in an emergent manner, and they are the result of the interactions acting between the components of the system. These patterns appear and change in their statistical characteristics by modifying the relevant parameters of the system like: temperature, density, coupling strength between the components , etc… Many times they are accompanied by phase-transitions, or they are signs for a critically self-organized state. Our group was quite active in the last few years in modeling and understanding a huge variety of emergent phenomena where surprising spatio-temporal patterns were observed. We have studied synchronizing oscillator ensembles [1-8], structures emerging from capillary phenomena [9-11], self-organization of atoms and nanoparticles on solid surfaces [12,13], structures emerging from fracture or fragmentation [14-17]. We have considered interdisciplinary applications as well, describing patterns of human mobility [18,19], fluctuations in stock prices and stock-indexes [20,21], patterns in wealth and income distributions [22,23] and diversity patterns in neutral-like biological communities [24,25]. Parallel with the analytically tractable models, we have considered computer simulations with Molecular Dynamics or Monte Carlo methods to understand such phenomena. Data was collected by modern data-mining and processing techniques, and for some problems we have also constructed simple experimental apparatus and automated data acquisition systems. Nowadays this research field is in the spotlight of statistical physicists, and many new ideas and interdisciplinary problems are considered. Due to its interdisciplinary character, the ambitious aim of describing such patterns raises new challenges to physicists. Many times the classical models and methods of physics have to be modified and made more complex in order to deal with the higher level of complexities encountered in biology and socio-economic phenomena. Nevertheless approaches by simple and few parameter models are still welcome, since in such approaches one can test the validity of some basic hypothesis and make a hierarchy on the importance of different factors. Many complex patterns have root in the very same universal phenomena, and by understanding them through a unified model we discover the main driving force that leads to their appearance. In this aspects re-iterating the older and fundamental model families and looking for a wider class of phenomena that can be described by them is one priority for the researchers working in this field. The present project aims to investigate two such classical models of statistical physics: the Kuramoto type model and the depinning type models. These models will be reconsidered in new perspectives and by having in our view new interdisciplinary application possibilities. Beside these two models we plan to model and understand another interesting socio-economic phenomena: mobility patterns generated by the travel of commuters.

D2. Objectives

The first problem that will be studied is a natural continuation of our research in the field of spontaneous synchronization of Kuramoto type oscillators, focusing on a timely and newly discovered phenomena: the presence of *generalized synchronization states* and *chimera* type states. Collective behavior in ensembles of interacting oscillators is one of the oldest problems in the field of dynamical systems and statistical physics [26,27]. Interestingly however, this field is still active, raising new problems [28], revealing further surprises [29] and offering applications and modeling tools for many other areas of science and engineering [30]. Synchronization of non-identical and coupled oscillators is an intriguing fact observed in many real systems. The Kuramoto model is probably the most widely studied system for modeling such synchronization phenomena. For globally coupled rotators it exhibits an order-disorder transition, which is useful to explain emerging synchronization in physical, social or biological systems [31]. By varying the characteristics of the interactions acting between the rotators, many variants of the original model were studied analytically and numerically. It was found that the topology of the interaction determines the nature of the emerging collective behavior. In such sense the Kuramoto model was considered both on regular and random graphs using interactions between neighbors of different order [31]. The model was generalized also by considering a mixture of attractive and repulsive couplings. In general, for locally coupled non-identical oscillators it was found a rich variety of collective behavior: frequency locking, phase synchronization, partial synchronization or incoherence. Time-delay in the interactions between the active neighbors introduces an extra complexity in the Kuramoto model by drastically increasing its dimensionality [28,31,32]. The model becomes also more useful for describing real physical phenomena [33]. Even for two Kuramoto rotators coupled with a time-delay, a multitude of synchronized solutions are emerging [34]. It yields also new surprises in large oscillator ensembles, by generating novel, long living transient states where some of the oscillators synchronized while the others remained completely disorganized. Such states were named as "chimera" states, and they were observed in many different coupling topologies [28,29,35]. These intriguing states were recently reproduced also experimentally [36]. Nowadays it is believed that the condition to get such "chimera" states in interacting oscillator ensembles is to have local interactions extending to several neighbors and time-delay in the coupling. Even systems of identical oscillators can end up in chimera states. Here we will continue this line of studies by considering a one-dimensional circular ring of identical Kuramoto oscillators with uniform time delayed interaction between the neighbors. Based on earlier studies in such systems [32,33] we expect to get several types of stable collective states, or different synchronization modes. For nearest-neighbor coupling one observes rotating waves and also the fully synchronized, in-phase state. It is interesting problem is to find the appearance probability of the different states if the system is randomly initialized. One would be also interested how the probability distribution of the final stationary states can be modified by changing the system's relevant parameters. Such problems are open question nowadays, and a detailed stability analysis or computer simulations could offer a satisfactory answer. A first step we will have to do is to define proper generalized order parameters that are easy to follow in computational studies. Another crucial step will be to generalize the classical stability analysis know for dynamical systems to systems with time-delay. After elucidating the problem of the generalized synchronization states, the second question we are interested in is to find what interaction kernel is needed in order to obtain the chimera states that are nowadays in the focus of such research. Making again a detailed computer simulation study could shed more light on these intriguing phases. For the ring-like system one can construct then a simple phase-space diagram indicating the different synchronization phases that are expected in the dynamical equilibrium as a function of the system parameters. Beside the described theoretical approach in this research problem we would also like to find physical and socio-economic examples of real-life phenomena where these generalized synchronization or chimera states appear. One immediate candidate is the synchronization-like phenomena that are observed in the response of the crowd (blowing vuvuzela, making Mexican waves or just encouraging the team) in large open-air stadiums where the delayed and localized coupling conditions are fully satisfied. Another example can be neuron or pace-maker type cell in our body.

The second problem we would like to consider in the framework of this project deals with some intriguing statistical laws that one can find while studying human travel. Recently we have shown for example that the travel distance and average traveling speed connects through a puzzling nonlinear scaling relation [18]. Here we plan to address a long standing problem in the field of human mobility, namely, how the travel (or commuting) fluxes starting from a given city decreases with the travel distance. Several studies were concerned in finding out the specific form of this relationship [37] and beginning with the mid XX century, scientist considered many modeling attempts also. In the beginning phenomenological models borrowed from physics (like the *gravitational type models* or the *generalized potential models*) were used [38,39] to describe the travel flux-distance relationships. It turned out the travel flux data between cities can be reasonably well described with a relationship, resembling the gravitational law and a general fitting from of the type: works well. Here is the population of the starting city, is the population in the target city and r_{12} is the distance between them, $K, \alpha_1, \alpha_2, \beta$ are fitting constants. Beside this simple form other even more complicated fitting forms were proposed. Due to the large number of fitting parameters it is not surprising that one can describe the experimental results fairy well. Recently Simmini et. al [40] has taken another approach. Rather then considering more complicated fitting forms, they proposed to start from "first principles" and building a theoretically well-motivated simple model. Their model named as the "*radiation model*" results in a very simple formula, implying that the probability that a commuter transits over a number a of closest job openings is: $P_>(a) = 1/(1+a)$. Assuming that the number of job openings in a territory is proportional with the population W ($a = \alpha W$), this formula leads to a very simple approximation with one fitting parameter for the commuter fluxes. Interestingly, this simple formula works well for describing the commuter's fluxes in USA. This simple approach was theoretically better founded by our work [19], considering a mathematically generalized continuum approach to the problem. Our more realistic model, named as *radiation model with selection*, gives a two-parameter result for the same probability: $P_>(a) = (1-\lambda^{a+1})/[(1-\lambda)(a+1)]$, where λ is a parameter between 0 and 1 and gives the probability to accept any job offer that pays better than the closer ones. In such case one obtains for the fluxes a two parameter fit as a function of the transited population. This modified formula leads to even better fits for the commuter fluxes in USA, and the traveler fluxes determined from mobile-phone log-data [19]. In this new picture, seemingly for understanding the commuting patterns not the distance is the important quantity, but rather the transited population. Recently however, we have studied experimentally commuter patterns in Romania and Hungary, and found that none of the classical models offer a good fit for the experimental data. Moreover, we observed a non-trivial dependency of the commuting patterns on both the distance, r, and transited population, W. In the picture offered by the new experimental results we believe that a good approach for describing the commuter patterns would need a newer model, where both the distance and transited population are taken into account. Our aim here is to develop such a model, and to verify the model prediction on the empirical data for Romania and Hungary. This research would involve in such manner analytical calculations, similar to the one considered in [19], and numerical methods for comparing the model results with one obtained from commuter data in Romania and Hungary. The generalized patterns of commuting as a function of both distance and transited population are also interesting by them self, and one could make comparative studies between different regions in a country or even different countries.

The last research topic we would like to consider within this project concerns problems related to depinning. The motion of interfaces in a disordered potential is a ubiquitous phenomenon in physical systems. As examples, we can mention the motion of dislocations [41] or magnetic domain walls [42] in a crystal with impurities, crack front propagation in a material with inhomogeneous toughness [43] or the motion of a dewetting front on an inhomogeneous substrate [9]. In all of these systems the dynamics is a result of the competition between the disorder and the elastic interactions along the interface: local minima of the disordered potential tend to pin (trap) the interface, whereas elastic forces tend to flatten the interface. As a result of the interplay between elasticity and disorder, the interface follows a jerky, stick-slip dynamics. At vanishing velocity, we encounter critical properties: avalanche events, long range correlations, scaling properties etc, showing that such depinning systems exhibit a dynamic phase transition. Recently we extended the standard depinning model to capture the large deformation regime of a receding dewetting contact line [9]. We elaborated a new and very efficient computer simulation method for modeling the dynamics of the contact line, which is applicable also for a strongly inhomogeneous surface. Our method is a mesoscopic-scale molecular dynamics method, where the interface is discretized with virtual characteristic points. Applying a Hamiltonian approach we write the equations of motions for these characteristic points, and integrating these we follow the dynamics of the interface. Applying the method on a model surface with randomly distributed point-like pinning centers we found the existence of a new propagation regime that is governed by the tearing up of the layer, as well as critical properties at a threshold concentration or threshold strength of the substrate inhomogeneities. In the critical regime the contact line exhibits also a critical roughening showing fractal-like structures. Here we aim to further extend the model to study the dynamics and the stationary morphology of the contact line on patterned surfaces. Unlike in our previous study [9], we propose a regular placement of surface inhomogeneities and adjust the strength and the distance between the pinning inhomogeneities. Moreover, we will carry out both simulations and experiments with such a patterned arrangement. As a first trial the simplest geometry, of inhomogeneities will be considered, where the pinning centers are distributed on the sites of a square lattice. Experiments will be done with a carefully prepared metal plate in which regular holes will be drilled and filled with paraffine. Simulations will be done on the cluster of our group while the experiments will be done in collaboration with the physical chemistry department of the University of Szeged, Hungary. We expect to prove experimentally the existence of the depinning transition, to show the influence of the density of the impurities and to study also the influence of the layer thickness. Understanding and controlling the dynamics of thin layer dewetting is not only a theoretically challenging problem, but it is also of great industrial interest as the contraction of thin layers is the main limitation in various coating processes [44]. In such sense we feel that also this pattern formation problem has an important practical applicability.

D3. Impact

We consider that all the problems that will be studied in the proposed project are of large interest for a broad scientific community. The synchronization problem deals with the recently discovered chimera states, which is in the center of attention for a broad community of statistical physicists. Understanding puzzling, rotating-wave-like synchronization patterns is also a fundamentally important problem with potential applications in biology, chemistry and even social sciences. Ring-like setups of oscillators can be a new and easy way of making oscillator system with tunable frequencies or for engineering more stable and error tolerant oscillator devices. The commuting problem and the puzzling patterns that is present there are naturally of interest for both, economists, geographers and sociologists. We believe that this problem has an even broader interest, since even the scientifically untrained public is interested in finding out the characteristic commuter patterns that influences our everyday travel and business. This problem has a clear interdisciplinary character where statistical physics can show again its usefulness for tackling problems that involve a large number of interacting elements. The third problem considered in this proposal has a clear industrial relevance, since the dewetting process is present in many processes where thin coatings with different properties are placed on surfaces. On one hand industry is sometimes interested in the wetting process to form uniform thin layers on various surfaces, but on the other hand for some applications the dewetting problems is the one that we want to avoid or to enhance. Apart from the interest from industry, the depinning transition is a dynamical phase-transition accompanied by critical phenomena. Statistical physics is thus naturally interested in understanding such phenomenon and to learn more about the critical behavior that is present at the transition point. We also consider that the research problems that will be studied have an importance in training PhD students. The PhD students that are involved in this project will get thus an interdisciplinary training and the big variety of considered problems will offer them a choice for freely choosing the research project according to their scientific interests.

D4. Methodology

The project focuses on three clearly defined problems, all of them dealing with spontaneously forming spatio-temporal patterns. They all have a modeling part that will be approached mostly by computer simulations. The models that we have in mind and were detailed previously are not analytically solvable so either Molecular Dynamics simulations or Monte Carlo type methods will be used. For the time-delayed synchronization problems and the study of the chimera states, the computational modeling approach will be complemented by analytical approaches that are considered to be classical in the theory of dynamical systems. Theories of critical phenomena and scaling theory will be used to discuss the phase-transitions that are expected in the system of coupled ring-like systems. The human mobility project needs data mining and experimental data processing to reveal the phenomenological trends. The data we will process on commuter's fluxes are available to us through the most recent census data in Hungary and Romania, and they are provided through our personal professional connections with researchers working in the Central Statistics Office in Romania and Hungary. This data is processed by computer codes that will be written by our team. Modeling will be done using the same analytical methods that were used by us in [19]. In case the complexity of a successful model requires a computational modeling, we will do also computer simulations and numerical studies. For the problem of the depinning transition in the dewetting problem we will collaborate with a team specialized in experiments, leaded by Dr. Bogya Erzsébet from the Physical Chemistry Department of the University of Szeged, Hungary. Experiments will be done in their laboratories and the video-recorded data will be processed in our computational laboratory at the Physics Department of the Babes-Bolyai University. Computer modeling for the dewetting model elaborated by us [9] and properly adapted for the specific experimental setup will be done on the computational cluster of our group. These are Molecular Dynamics and Monte Carlo type simulations that are straightforward in the context of the general computer code that was previously developed by us. We hope that our dewetting model will be capable of reproducing qualitatively the observed experimental trends.

The **diagram 1.** (see next page) details our work plan, the organization of the research in relation with the proposed objectives, the potential risks and the undertaken deliverables. Please note that the research in all three problems will run in parallel.

D5. Ethical aspects (if appropriate)

The census data for Romania and Hungary does not contain any private information for the commuters like names, personal numbers, birth date, exact address, etc... In such sense the data does not present any concerns for violating privacy. Due to the fact that the dataset is the property of the Central Statistical offices from Romania and Hungary we will not distribute the rough data, just the processed data of our research.

Task Name	Start Date	End Date	Methods/Activities	poter
studies on the Kuramoto-type systems	**01/01/17**	**03/01/19**		
computational studies for the probabilities of different synchronization states	01/01/17	05/01/17	model construction, programming, computer simulations	-
analytical studies on the stability of different states	05/01/17	08/01/17	analytical calculations	- migh analyt compa (!)
concluding the results for the stability of different rotating waves	08/01/17	10/01/17	writing up the results, presenting at conferences, sending for publication	-
computational studies on chimera-like states	10/01/17	07/01/18	model construction programming, computer simulations	-
studying the phase-space of different collective behavior as a function of relevant system parameters	07/01/18	01/01/19	data processing, graphical presentation of the results	- migh very a phase- structu
concluding the results on chimera-like states	01/01/19	03/01/19	writing up the results, presenting at conferences, sending for publication	-
studies on commuting patterns	**05/01/17**	**08/01/18**		
census data processing and graphical presentation of the commuting patterns	05/01/17	09/01/17	data mining, data processing	-
elaborating a new model for travel flux	09/01/17	03/01/18	modelling, analytical calculations, computer modelling	- migh in a co comm formu
testing the model	03/01/18	05/01/18	computer simulations	-
concluding the results	05/01/18	08/01/18	writing up the results, presentations at conferences	-

diagram 1: work plan spread in time, potential risks and expected deliverables

D6. Resources and budget

The research group: The proposed research group has four senior researchers one post-doc and two PhD students. The director of the project who will also be the key researcher of the team, **Professor Dr. Zoltán Néda** has a strong background in statistical physics and computational physics. His actual research area is the field of collective behavior with original applications both in physics, biology and socio-economic problems. He authored more than 93 ISI papers and for these works he received more than 2100 independent ISI citations. The other group members are constant collaborators of Prof. Néda. **Assistant professor Dr. Ferenc Járai-Szabó** is an expert in computational physics and master both the Molecular Dynamics and Monte Carlo type simulations. He authored many works in the field of stick-slip type dynamics in spring-block models, pattern formation in complex systems and numerical methods in atomic physics. **Assistant Professor Dr. Arthur Tunyagi** is physical engineer who has a strong research record in building computer interfaces and connecting sensors to experimental setups. He designed many experiments for the team of Prof. Néda. Together with **Assistant Professor Dr. Susana Sárkozi**, who has a background in experimental fluid mechanics and magnetism, they will provide help in realizing the experiments, automatic data collection and data processing. **Dr. Botond Tyukodi** who will be a post-doc researcher in the team has recently defended his PhD thesis in the field of depinning models (joint supervision between Z. Neda and D. Vandembroucq, UBB and Univ. Pierre et Marie Curie, Paris). He will be in charge with writing the simulation codes for the dewetting problem. The team will have also two PhD students, both of them students of Professor Néda. One of them is already in the PhD program: **Drd. István Papp.** He has excellent programming skills and worked already in problems related to human travel. The other student we have in perspective (open position) is **Mr. Károly Dénes**, currently graduating the computational physics masters section, and who worked in his master thesis in the field of spontaneous synchronization in time-delayed Kuramoto models. He intends to apply for a PhD position in the team of Prof. Néda.

Computational resources: Our group has a modern and strong parallel computational cluster with more than 128 nodes and more than 8GB of RAM per node

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http://www.erris.gov.ro/main/index.php?&ddpN=1693097241&we=d3cdf3482aed0446e2532b946e1769a8&wf=dGFCall&wtok=f235ef10616d5dbde0780dcd793c63a11e28a202&wtkps=dU/LDoIwEPyXvUtoS1O63DiY+BWm9KGNNQIFCTH+uy3K0dNOZiazMwolviJyhGW6hQiNR8ZKQZuIDCF6AxlRBF4xRUomad1VVEpHKDOM8LrSUjjjNl+yLTYDIhDuDzMHW6i+L6JVo75uAsKw3WRtVWfjoX2EVfmf9sz/y4QlQvBxOvfqYndO7FxqaTA3TK2H2Y7rv8SUot1RaR9O3x0INefQvD8=&wchk=232e22b2dcc60d789812c5667053454ac32936b8#s

Computer simulations will be realized on this cluster and on the new IBM supercomputer that was recently installed in our University. The group has also several servers on which Linux and MAC OsX operating systems are run. On this computers smaller computational problems are elegantly solved.

The proposed budget will focus on the following priorities:

1. Salaries for the research done by the team members have to be provided. One of our priorities is to ensure a decent salary also for the PhD students and for Dr. Botond Tyukodi, who will have a part-time post-doc position in the team.
2. Publication fee in open-access journals are included in the logistics expenses
3. Travel, registration and subsistence expenses to conferences and international collaborations are expected. These are included also in the logistics expenses.
3. The existing computational resources have to be updated by new nodes and new servers. Personal and laptop computers on which the team members are working have to be also updated. These will be included also in the logistic expenses.
4. Office supplies necessary for the work are also included in the logistics expenses.
5. The indirect overhead expenses (25%) required by our University has to be provided