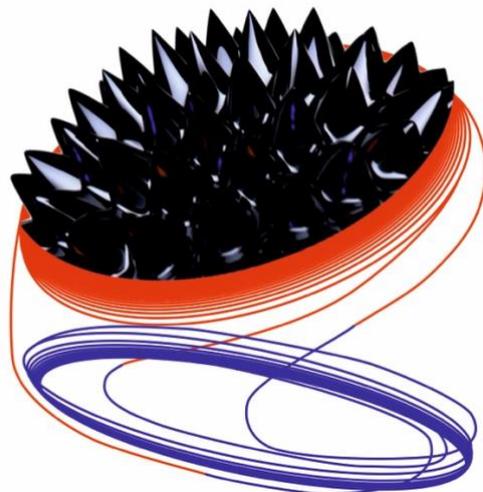


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# Stochastic sensitivity analysis: its relevance for economists

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Real existing economic systems have been observed to produce robust statistical pattern in key-state variables. The paradigm of stochastic non-linear dynamics can account for such distributional regularities arising from specific institutional, environmental, and behavioral postulates. Uncompromizing economic theorizing typically identifies essential *feedback loops* of the system which are subject to intrinsic and/or extrinsic *noise* leading to models that can be coded as stochastic non-linear differential or difference equations.

These models are known to give rise to a rich dynamic structure and a *cornucopia* of noise-induced phenomena which are highly relevant in the context of economics. Despite those facts, the propensity to embrace the results generated in this modelling environment is low, not only among policy makers but even among academic economists. One explanation simply lies in the technical complexity of the matter. Moreover, some analytical strategies implemented in the context of stochastic dynamics do not necessarily generate the information about the underlying system that academic economists and policy makers rely on. Their informational needs derive from the technique of *comparative statics* traditionally used to assess an economic equilibrium.

We demonstrate that *sensitivity analysis* due to [1, 2], as well as its various spin offs, can be viewed as an adaption of the comparative statics approach to a complex dynamic stochastic setting. Drawing on some of our past work, as well as on work in progress, we exemplify how the stochastic sensitivity function technique can be put to work to answer the questions typically held by a research economist and/or a policy maker who works with a stochastic non-linear economic model. In our discussion, special emphasis is given to the phenomenon multi-stability.

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# Noise-induced oscillatory activity in the 3D model of cold-flame combustion of a hydrocarbon mixture

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We consider a stochastic model of cold-flame combustion of a mixture of two hydrocarbons in a flow reactor [1, 2]. The initial deterministic model is a three-dimensional system of nonlinear ordinary equations: two variables describe the concentrations of two reagents, and the third variable denotes the temperature. The model is characterized by a presence of multiple equilibria, hysteresis zones and self-oscillations. We study an influence of noise on the model in the parametric zone of monostability, where the only attractor of a deterministic system is a stable equilibrium. We show that in this case, random disturbances can induce large-amplitude oscillations. Using numerical simulations, we obtain statistics of spatial and temporal characteristics of emerging oscillations. By means of the analytical approach based on the stochastic sensitivity functions and confidence ellipsoids [3] we study the probabilistic mechanism of stochastic generation of oscillations.

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# Mathematical modeling and analysis of stochastic tumor-immune nonlinear dynamics

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Mathematical modeling and analysis of dynamic processes in different areas of biology is the one of the most important problems in modern nonlinear science. We study a two-dimensional model of the dynamic interaction of tumor and immune cells under conditions of chemotherapy and random effects:

$$\begin{cases} \dot{x} = \sigma + \rho \frac{xy}{\eta + y} - (\mu + \varepsilon\xi(t))xy - \delta x; \\ \dot{y} = \alpha y(1 - \beta y) - xy - \frac{by}{1 + y}. \end{cases}$$

This model is an extension of the well-known Kuznetsov's model [1]. Here,  $b$  is a coefficient of chemotherapy intensity,  $\xi(t)$  is random noise. This modification leads to the emergence of new modes of dynamics. The report presents the results of a bifurcation analysis of the deterministic model depending on the chemotherapy intensity parameter  $b$ . It has been shown that the system admits different characteristic states for different values  $\mu$ : a “dormant” tumor, which is represented by equilibrium and oscillatory modes or only equilibrium modes, “zero” tumor and “active” tumor. For equilibrium and oscillating regimes, we found the parametric zones of coexistence and separatrices, which share the basins of the corresponding attractors. Also, we found the estimates of the coefficient of chemotherapy intensity of transition to the state of “zero” tumor.

For the stochastic model, scenarios of the effect of random fluctuations on the modes of dynamic interaction between immune and tumor cells are described. The conditions under which noise-induced transitions between attractors occur are studied. For the stochastic model we found conditions under which random fluctuation play a positive role, reducing the number of tumor cells.

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# Noise-induced generation of spatial patterns in glycolysis

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The problem of spatiotemporal self-organization in reaction-diffusion models attracts the attention of many researchers. Turing instability is a well-known cause of the generation of spatially inhomogeneous patterns in a wide range of diffusion models [1]. It is well known that any real process is inevitably affected by random noise caused by the environment. The aim of this work is to study the constructive role of noise in the processes of self-organization in glycolysis.

Spatially distributed Selkov's glycolytic model [2,3] with diffusion is considered. Multistability of this model is discussed, and the variety of patterns is described. A phenomenon of noise-induced pattern formation in the zone of Turing stability is studied. We carry out a statistical analysis of the effect of noise on the process of pattern formation and determine the stochastic preference.

For the analysis of the processes of pattern formation, the method of harmonic coefficients is applied. Statistical properties and stability of noise-induced patterns are discussed. A comparison of noise-induced pattern formation in different parametric zones is performed.

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# Analysis of stochastic multistable consumer behavior model

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The paper considers a stochastic version of the discrete model that describes the dynamics of two consumers interaction [1]:

$$\begin{aligned}x_{1t+1} &= \frac{b_1}{p_x p_y} (a_1 x_{1t} (b_1 - p_x x_{1t}) + D_{12} x_{2t} (b_2 - p_x x_{2t})) + \varepsilon (\xi_1 \sigma_1 + \xi_3 \sigma_3 \frac{b_1 D_{12}}{p_x p_y} x_{2t}), \\x_{2t+1} &= \frac{b_2}{p_x p_y} (a_2 x_{2t} (b_2 - p_x x_{2t}) + D_{21} x_{1t} (b_1 - p_x x_{1t})) + \varepsilon \xi_2 \sigma_2.\end{aligned}\quad (1)$$

Here,  $x_1$  and  $x_2$  are units of goods consumed by the first and second individuals depending on time  $t$ ,  $p_x$  and  $p_y$  are the cost of goods  $x$  and  $y$ . Parameters  $b_1$  and  $b_2$  determine the constant income of the first and second individuals. Parameters  $a_1, a_2$  and  $D_{12}, D_{21}$  are referred to as *learning* and *influence* parameters respectively.

The paper studies the parametric domain  $(D_{12}, D_{21})$  in which the deterministic model demonstrates complex dynamics with zones of coexistence of various attractors. Particular attention is paid to the regions of coexistence of up to 5 attractors. Bifurcation scenarios and basins of attraction are studied. We also consider an example when one of the attractors of the system synchronizes the variables  $x_1$  and  $x_2$ .

In the case of the impact of a random perturbation of two types (additive and parametric noise), noise-induced transitions between attractors are studied, and dominant attractors are identified. The phenomenon of desynchronization caused by a random disturbance is described. For a constructive description of stochastic phenomena, the stochastic sensitivity function technique and the associated confidence domain method are used [2].

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# Analysis of stochastic phenomena in the hierarchical Bazykin-Aponin model

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The paper studies the Bazykin-Aponin model [1] with the following hierarchical structure: two prey populations coexist and compete for food resources, and both populations serve as food for predators. Earlier this model was studied in [2,3]:

$$\begin{aligned}\dot{x} &= x(2.4 - x - 6y - 4z), \\ \dot{y} &= y(b - x - y - 10z) + y\varepsilon\xi(t), \\ \dot{z} &= -z(1 - 0.25x - 4y + z).\end{aligned}\tag{2}$$

A bifurcation diagram has been constructed, zones of coexistence of equilibrium, regular and chaotic oscillation modes of interaction of all three populations have been identified. In our study we focus on the multistable zone and investigate in detail the coexisting of two stable cycle with equilibrium.

The mechanisms of multistage stochastic transitions between regimes, which generate mixed mode oscillations and extinction of populations, are revealed. A constructive parametric description of the observed probabilistic phenomena is obtained using the stochastic sensitivity function and the method of confidence domains [4]. We also show the noise-induced chaotization and “order-chaos-order“ transition.

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# Patterns in distributed systems: Stochastic sensitivity technique

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Self-organization dynamics in complex non-linear models is currently one of the most attractive fields of research in natural sciences [1-4]. One such case of study is the self-organization in population dynamics. In such models the diffusion instability phenomenon is observed – the spatially homogeneous state becomes unstable and stationary non-homogeneous patterns are generated.

The effect of random noise on the system dynamics and internal processes is an important aspect of research. In the presence of random perturbations various noise-related phenomena are observed. One such example is the stochastic transition between coexisting patterns-attractors [5]. Such transitions imply difference in stochastic sensitivity of these patterns. An in-depth investigation of pattern stability is currently an actual research problem.

In this report a spatially extended population dynamics model is considered. Multistability of the model in the diffusion instability zone is demonstrated. The distribution of random states around a stable pattern-attractor is estimated using the stochastic sensitivity function (SSF) technique. The variation of stochastic sensitivity of coexisting patterns depending on system parameters is shown. Basins of attractions of these patterns are studied for varying system parameters. Using the data obtained from numerical modelling the relation between the stochastic sensitivity, the boundaries of the basins of attraction and stochastic transitions is discussed.

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# Stochastic variability in metapopulation dynamics

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Consider stochastic system of two coupled population subsystems modeled by the Ricker map [1]:

$$\begin{cases} x_{n+1} = x_n e^{\mu_1(1-x_n)} + (\sigma + \varepsilon \xi_n)(y_n - x_n), \\ y_{n+1} = y_n e^{\mu_2(1-y_n)} + (\sigma + \varepsilon \xi_n)(x_n - y_n), \end{cases} \quad (3)$$

where  $x$  and  $y$  are population sizes,  $\mu_1 = 1.8, \mu_2 = 3$  are parameters of the intrinsic growth rate,  $\sigma > 0$  is a coupling coefficient, characterizing the intensity of mutual flows between two population subsystems,  $\xi_n$  is Gaussian noise, and  $\varepsilon$  is the noise intensity. The first isolated subsystem is in equilibrium state, and the second one is in chaotic state. A detailed stochastic analysis of regular and chaotic dynamics in the case of two equilibrium isolated subsystems was carried out in [2].

The purpose of this study is to analyze the modes of corporate dynamics of metapopulation consisting of equilibrium and chaotic subsystems. The attractors of the deterministic system are presented and studied, the analysis of oscillatory modes of given population subsystems is carried out, basins of attraction for coexisting attractors are constructed for the corresponding values of the coupling intensity. A stochastic system that takes into account the influence of random perturbations is considered in detail. Using the stochastic sensitivity function method, stochastic phenomena that give rise to new modes of population behavior are studied: transitions induced by noise from one regular attractor to another, from order to chaos and vice versa.

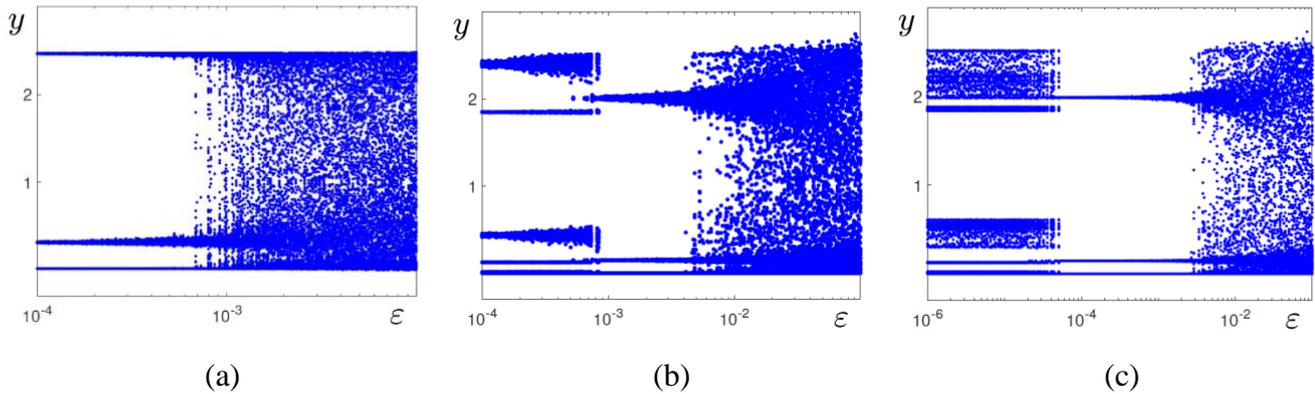


Figure 1 – Noise-induced transitions in system (1): random states versus noise intensity

In Fig.1 noise-induced transitions are shown for the different values of the coupling parameter  $\sigma$ :

(a) “3-cycle  $\rightarrow$  chaos” for  $\sigma = 0.01$ ; (b) “6-cycle  $\rightarrow$  3-cycle  $\rightarrow$  chaos” for  $\sigma = 0.141$ ; (c) “chaos  $\rightarrow$  3-cycle  $\rightarrow$  chaos” for  $\sigma = 0.138$ .

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# Synthesis of stable dynamical modes in stochastic systems with incomplete information

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At present, the theory of control of dynamical systems is an actively developing scientific field with important engineering applications. Accounting an influence of inevitably present random perturbations complicates the formulation of control problems and initiates the development of new adequate methods of the stochastic analysis and synthesis. The constructive technique of stochastic sensitivity functions, which makes it possible to approximate distribution densities near attractors has been successfully used in the analysis of various kinds of stochastic phenomena [1]. In solving problems of synthesis for controlled stochastic nonlinear systems, the stochastic sensitivity method is also helpful [2,3].

In this talk, a problem of the synthesis of the assigned stochastic sensitivity for equilibrium modes in nonlinear dynamical systems with random perturbations and incomplete information is considered. For the feedback matrix of regulator, a quadratic equation is derived, which connects its parameters with the assigned stochastic sensitivity. The questions of attainability are investigated and an algorithm for solving this equation is carried out. These general results are used to solve the problem of stabilizing equilibrium modes of nonlinear oscillators under conditions of incomplete information. Efficiency of the suggested approach and elaborated mathematical technique is illustrated by the example of the solution of stabilization problem for stochastically forced van der Pol oscillator.

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# Methods and algorithms for approximation of probabilistic distributions of stochastic attractors

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Mathematical models in the form of nonlinear differential or difference equations with random disturbances are widely used to study dynamical processes observed in different areas of science. The interrelation of nonlinearity and stochasticity often leads to new phenomena that have no analogues in the original deterministic models. Direct numerical modeling remains the main tool for studying such nonlinear stochastic phenomena. Within the framework of this extremely costly method, it is difficult to obtain clear parametric descriptions of various stochastic regimes of the models under study. In order to carry out a detailed parametric analysis of probabilistic mechanisms of these new stochastic phenomena, the development of analytical approaches is required.

In this talk, we focus on the study of randomly forced discrete-time dynamical systems and give an overview of the new constructive approach for the approximation of randomly forced attractors. Our approach is based on the stochastic sensitivity analysis developed for equilibria, cycles, closed invariant curves, and chaotic attractors of discrete-time mathematical models. Using this technique, we elaborate an approximation of probabilistic distributions in the form of confidence domains. Constructive abilities of suggested analytical approach are illustrated for diverse stochastic phenomena in discrete systems with quadratic map and coupling.

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# Ferrofluids and bio-ferrofluids: looking back and stepping forward

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Ferrofluids investigated along about five decades, are ultrastable colloidal suspensions of magnetic nanoparticles, which manifest simultaneously fluid and magnetic properties. Their magnetically controllable and tunable feature proved to be from the beginning an extremely fertile ground for a wide range of engineering applications. More recently, biocompatible ferrofluids attracted a huge interest and produced a considerable increase of the applicative potential in nanomedicine, biotechnology and environmental protection. This paper offers a brief overview of the basis achieved in the studies of these complex systems including their synthesis and elaborate characterization, as well as a recent progress in multifunctional materials derived from ferrofluids and their applications based on the ferrofluid-driven assembly and manipulation technologies.

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DOI: 10.1039/D1NR05841J

# Динамика многофазных систем на основе магнитных жидкостей: эксперимент и моделирование

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Магнитные жидкости обладают уникальным сочетанием магнитных свойств, текучести и коллоидной стабильности, что позволило им найти применение в различных технических устройствах. Одной из особенностей этого умного материала является возможность управлять его физическими свойствами с помощью различных комбинаций магнитных воздействий. Возможности «классических» магнитных жидкостей могут быть значительно расширены путем добавления одной или нескольких дисперсных фаз, в качестве которых могут выступать пузырька газа, капли несмешивающихся жидкостей, а также твердые магнитные и немагнитные включения. Комбинированные внешние воздействия на подобные многофазные магнитные системы при различных вариантах течений позволяют добиться управляемой динамики как в каналах миллиметрового размера, так и в микроканалах, что представляет несомненный интерес для микрофлюидики, где привычные способы управления потоками не работают.

Показано, что размер образующихся немагнитных включений в такой магнитожидкостной системе не зависит от расхода и гидростатического давления. Возможность управления размерами немагнитных жидких и газовых включений путем изменения параметров магнитной жидкости и магнитного поля может быть использована для микродозаторов или счетчиков газа в микрожидкостных системах [1].

Также в данной работе исследуется динамика объема магнитной жидкости, левитирующей в однородном магнитном поле электромагнита, испытывающего колебательный сдвиг. Рассмотрены образцы с различными физическими параметрами, исследована зависимость магнитовязкого эффекта. Показано, что наибольшее влияние на динамику магнитной жидкости, испытывающей колебательно-сдвиговое и магнитовязкое воздействие, оказывают микроструктура образца и наличие крупных магнитных частиц. Результаты работы могут быть использованы для разработки метода экспресс-тестирования образцов магнитных жидкостей, а также для разработки датчиков ускорения и вибрации на основе магнитных жидкостей [2,3].

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# Thermal convection of magnetic fluid in a thin rectangular cell under the action of uniform magnetic field

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Natural convection is the main mechanism of heat transfer in many natural and technological processes, which makes it urgent to study the possibilities of controlling it. In this work, the processes of development and damping of thermal convection in a flat vertical quasi-two-dimensional layer of magnetic fluid are considered. The presence of the magnetic properties of the fluid makes it possible to effectively apply the external magnetic fields to regulate convective heat transfer.

In our experiments, we used a water based electrostatically stabilized magnetic fluid and a kerosine based sterically stabilized magnetic fluid with dispersed magnetite nanoparticles of about 10 nm in size. The magnetic nanofluid formed a layer with a horizontal length of 8 cm, a vertical length of 1 cm, and a thickness of 2 mm. Below and above the layer was bounded by aluminum plates. The magnetic fluid layer was heated from below.

It was shown that the imposition of an external uniform stationary magnetic field perpendicular to the temperature gradient leads to the suppression of convection (Fig. 1).

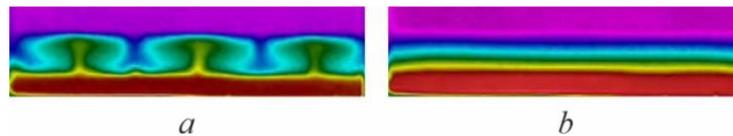


Figure 2 – Thermal convection pattern in a rectangular cell filled with a magnetic fluid. *a* – In the absence of a magnetic field. *b* – Under the action of a uniform constant horizontally oriented magnetic field.

The processes of heat transfer in a magnetic fluid are studied. The Nusselt number time dependence and the dependence of Nusselt number on Rayleigh number have been measured. It is shown that the suppression of convection by a magnetic field leads to a decrease in the total heat flux.

Numerical modeling of the processes under study based on the volume of fluid method was performed. It was shown that the experimental data and simulation results are in qualitative agreement. The obtained results can be considered as a model for understanding similar exchange processes in liquids under the action of magnetic field.

# Shape and break-up of viscous miscible 2D magnetic fluid drops in macro- and microfluidics

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The ability to control the dynamics of droplets of miscible fluids is of great importance for industries such as the chemical industry and microfluidics. The use of a magnetic fluid as a dispersed phase makes it possible to control this process using a magnetic field.

The dynamics and shape of a drop of a miscible magnetic fluid are studied. A kerosene-based magnetic fluid with density  $\rho = 1374 \text{ kg/m}^3$ , viscosity  $\eta = 0.176 \text{ Pa}\cdot\text{s}$ , initial magnetic susceptibility  $\chi = 2.1$ , and saturation magnetization  $M_s = 37 \text{ kA/m}$  was used. The ambient fluid is kerosene. Fluids were positioned in a Hele-Shaw cell with a distance between planes of 0.2 mm. The magnetic field lies in the plane of the cell.

It has been experimentally found and numerically confirmed that the development of the form of a miscible drop depends on the magnitude of the magnetic field. This is due to the fact that instability develops in that part of the droplet diffusion boundary that is perpendicular to the magnetic field. However, although the growth rate of short wavelengths is higher than that of long ones, their amplitude is smaller, and diffusion leads to their disappearance if the instability develops slowly. Therefore, as shown in [1], the final wavelength of the developed instability decreases with increasing magnetic field. In this regard, a variety of droplet shapes arises depending on the magnitude of the magnetic field.

The shape of the diffusion boundary of the drop changes with time: in a weak magnetic field ( $\sim 0.5 \text{ kA/m}$ ), the drop elongates very slowly, stretching along the field. In fields of the order of 5–7 kA/m, very small peaks first appear at the boundary, and then merge and form two large peaks. In fields of the order of 10 – 30 kA/m, the middle part of the drop remains almost unchanged, and elongation occurs only due to the tops of the drop, which elongate very quickly. In a strong magnetic field ( $\sim 90 \text{ kA/m}$ ), short-wavelength perturbations develop rapidly enough not to disappear due to diffusion. Therefore, numerous peaks appear at the tops of the drop, and the elongation of the drop along the magnetic field becomes chaotic.

The experimental results obtained qualitatively agree with the numerical simulation of a 2D drop by the finite volume method. An explicit scheme was used on a grid of  $2000 \times 3000$  nodes.

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# Physical and chemical sorption of oleic acid on a magnetite nanoparticle: experimental facts and quantum chemistry simulations

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Dynamic associates of colloidal particles in magnetic fluids of the "magnetite - oleic acid - kerosene" type are studied experimentally and numerically in the zero applied field. A general assumption about two possible variants of chemisorption: covalent and hydrogen bonds, - of surfactant molecules on magnetite particles is discussed (Fig. 1).

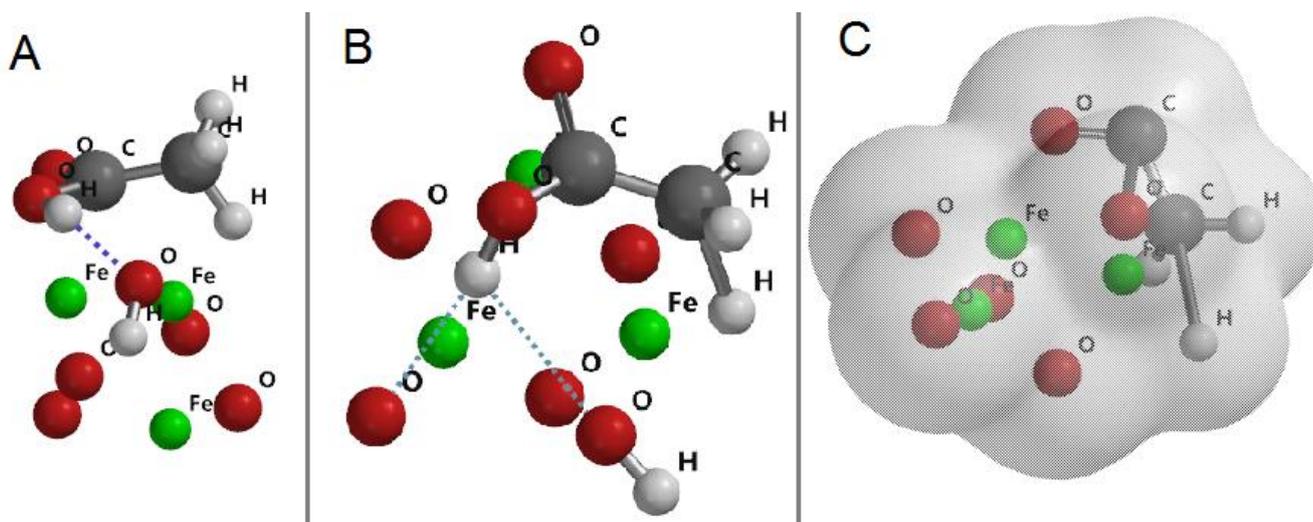


Figure 3 – Numeric simulation of acetic acid interaction with one  $\text{Fe}_3\text{O}_4$  “molecule” with the help of single (A) or double (B) H-bond (denoted by dotted lines), and with covalent bond (C). The opaque area in (C) denotes the electron density of the compound.

Gravimetric method is used to analyze colloidal particles extracted from ferrofluid samples subjected either to reversible flocculation caused by isopropanol at room temperature, or irreversible flocculation caused by boiling in acetone at 100 C. It is shown that 1-5 % percent of surfactant molecules are adsorbed by means of weak (physical) H-bonds, and thus can be detached from particles due to thermal motion. This result indirectly confirms the hypothesis about surfactant shell defects and explains dynamic association and peptization of particles forming quasispherical aggregates.

Computer simulations were carried out in Spartan [1] for just one “molecule” of magnetite  $\text{Fe}_3\text{O}_4$  and (thus the shortest possible) acetic acid. The simulations approve the possibility of the hypothesis and allow us to estimate the energy of both chemical bond types between real magnetite crystal and oleic acid surfactant molecules.

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# Chemical tailoring of the magnetic properties of core/shell nanoparticles

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The magnetic properties of nanoparticle assemblies are determined by a number of their characteristics, such as individual particles morpho-structural properties (i.e., size, composition, etc.) and properties of the whole particles system (i.e., particle concentration, matrix properties, etc.). Controlling such features, it is possible to design suitable magnetic properties of the materials for specific applications. This communication focuses on magnetic properties of the core/shell magnetic nanoparticles (MNPs) produced by high-temperature decomposition of metalorganic precursors with controllable structural properties [1,2]. One of studied systems is core/shell MNPs made of magnetically soft nickel ferrite and magnetically hard cobalt ferrite with different order of layers. An experimental study of the magnetic properties supported by computer simulations of the obtained systems (Fig.1) shows that the nanoparticle core has a determining role in the formation of magnetic anisotropy, while the shell material significantly modulates the surface properties. Moreover, we have shown how changing the individual magnetic properties of MNPs affects magnetic interparticle interactions and the magnetization reversal processes in their assembly.

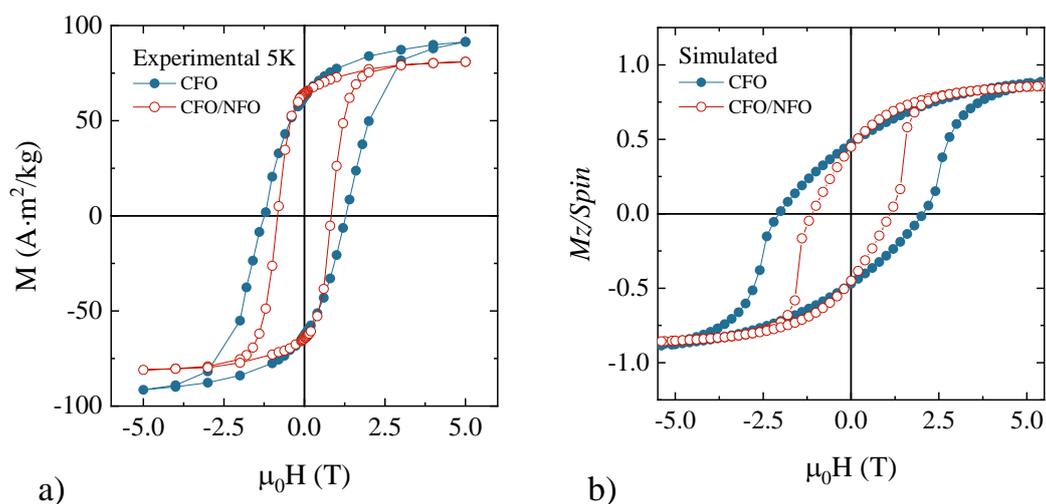


Figure 4 – a) M-H loops recorded at 5 K and inset is the low-field region at 300 K; b) Monte Carlo simulation results of the hysteresis loops for  $\text{CoFe}_2\text{O}_4$  and  $\text{CoFe}_2\text{O}_4/\text{NiFe}_2\text{O}_4$  particles.

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# Hydrodynamic and magnetic interactions in polymer-like structures.

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In this contribution we investigate supracolloidal polymer-like structures and magnetic nanogels under the influence of an applied magnetic field in a shear laminar flow.

First, we present a numerical study of the effects of monomer shape and magnetic nature of colloids on the behavior of a single magnetic filament subjected to the simultaneous action of shear flow and a stationary external magnetic field perpendicular to the flow. We find that based on the magnetic nature of monomers, magnetic filaments exhibit completely different phenomenology. Applying an external magnetic field strongly inhibits tumbling only for filaments with ferromagnetic monomers. The angle denoting filament orientation with respect to the flow direction is in this case independent of monomer shape. Alternatively, we demonstrate that reorientational dynamics exhibited by filaments with super-paramagnetic monomers, are not inhibited by applied magnetic fields, but enhanced. Spherical, super-paramagnetic monomers, depending on the flow and external magnetic field strength, relate to semi-persistent, collapsed, coiled up filament conformations. Tumbling frequency is a function of external magnetic field strength. However, external magnetic fields do not affect the tumbling frequency for filaments with cubic, super-paramagnetic monomers, but enhance its periodicity.



Figure 5 – Magnetic nanogel (a) and cube-based magnetic filament (b).

Next, we describe the impact of a shear rate on the shape, magnetic structure and motion of a magnetic nanogel (MNG). We find that in a shear flow the centre of mass of a MNG tends to be in the centre of a channel and to move preserving the distance to both walls. The MNG monomers along with translation are involved in two more types of motion, they rotate around the centre of mass and oscillate with respect to the latter. It results in synchronised tumbling and wobbling of the whole MNG accompanied by its volume oscillates. The fact that a MNG is a highly compressible and permeable for the carrier liquid object makes its behaviour different from that predicted by classical Taylor-type models. We show that the frequency of volume oscillations and rotations are identical and are growing function of the shear rate. We find that the stronger magnetic interactions in the MNG are, the higher is the frequency of this complex oscillatory motion, and the lower is its amplitude. Finally, we show that the oscillations of the volume lead to the periodic changes in MNG magnetic energy.

# Simulations of the Dynamic Magnetic Susceptibility of Magnetosomes

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Magnetosomes are found in magnetotactic bacteria, and consist of linear chains of tens of single-domain magnetic nanoparticles of Fe<sub>3</sub>O<sub>4</sub> (magnetite) or Fe<sub>3</sub>S<sub>4</sub> (greigite), enclosed in a lipid bilayer membrane. An example is shown in Fig. 1. The particles are typically in the size range 30-120 nm, and are practically monodisperse. Harnessing the power of biomineralization could lead to efficient strategies for synthesising semi-flexible dipolar filaments.

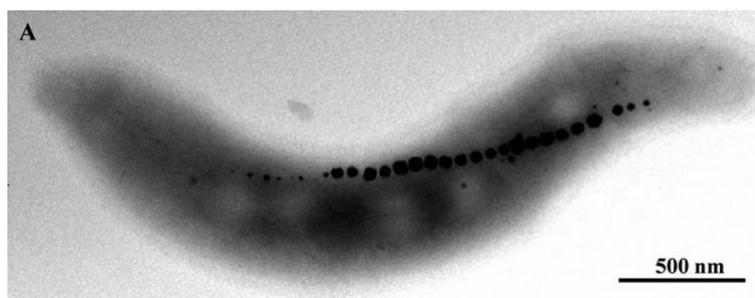


Figure 1 – Transmission electron micrograph of a cell of *Magnetospirillum magneticum* [1]

Brownian dynamics simulations of non-interacting magnetosomes, containing  $2 \leq N \leq 64$  ferromagnetic nanoparticles, have been used to determine their dynamical response to a weak AC magnetic field. The simulation model is shown in Fig. 2. Results are presented for the radius of gyration  $R_g$ , the dynamic magnetic susceptibility  $\chi(\omega)$ , and the effective Brownian rotation time  $\tau_B$ , all as functions of  $N$ . The results are compared to various theoretical predictions of the flexibility, susceptibility, and rotational dynamics of such magnetic filaments [2,3,4,5].



Figure 2 – Instantaneous configurations of model magnetosomes with  $N = 8, 16, 32,$  and  $64$

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# **A magnetoactive elastomer with magnetically hard filler prone to the particle/matrix adhesion break**

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Magnetoactive elastomers (MAEs), where a polymer is filled with micron-size ferromagnet particles come out now in different kinds. We discuss the MAEs based on magnetically hard (MH) particles, NdFeB in particular. Making, in fact, a new chapter in the MAE material science, these composites claim for a serious extension of the considerations applied to them.

In this context, the state and strength of the particle/matrix contact is an important issue. For the PDMS/NdFeB interface (typical case for real composites), a simple estimate shows that application of a field of a few hundred kA/m suffices to make an MH particle to get 'unleashed' and start to rotate relative to the wall of its cavity inside the elastomer. Remarkably, in the majority of theoretical works on these composites this possibility is completely ignored despite that the already accumulated experimental data: the magnetization loops of real MH-MAEs display the coercivities much lower than any estimates based on the Stoner-Wohlfarth model of the grains which constitute the particles.

Hereby, we report a model that explicitly takes into account the fact that the interface between the matrix and magnetic particles might break. In more detail: when a field is applied, it exerts a torque on the particle magnetic moment which, due to a high internal magnetic anisotropy, transfers it to the particle anisotropy axis, i.e., to the particle body itself. At relatively low torques, the particle responds reversibly and deviates from its initial orientation fully dragging on the surrounding matrix with it. As soon as the resisting elastic torque generated by the matrix exceeds some threshold, the adhesion breaks, the particle 'unleashes' and begins torsional slipping motion inside the cavity that it occupies. On the basis of that concept, we modify the description and, in result, arrive at a fairly good quantitative agreement with the magnetic measurements.

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# Dynamic remagnetization of a dimer of ferromagnetic nanoparticles

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Macroscopical properties and behavior of magneto-polymer composites are determined by combination of magnetic and mechanical characteristics of the embedded particles, the host medium, coupling between the medium and the particles, the particles spatial arrangement, etc.

Dynamical remagnetization of biological tissues with magnetic nanoparticles play a key role, for instance, in the effect of magnetic hyperthermia; it also presents interest from the viewpoint of development of technology of magnetically -controlled scaffolds of tissues engineering and regeneration

Some models of dynamic susceptibility of a system with chaotically (gas-like) distributed single domain ferromagnetic particles, immobilized in a host medium, recently were proposed in [1,2]. However, in the real systems, because of the magnetic, Van der Waals and adhesion interparticle interactions, the particles very often form various heterogeneous structures. Appearance of these structures can significantly affect the macroscopic response of the system on the applied field. Because of diversity of these structures and clusters, a general mathematical model for all their types hardly can be proposed. The most reasonable and realistic way is to consider the different types of the clusters separately. In this work we consider a simplest example of the cluster, namely - dimer consisting of two single-domain ferromagnetic particles immobilized in a carrier medium. Despite the physical simplicity of this approach, the results, obtained for the dimer, as well as the way of the cluster mathematical study can be a robust basement for consideration of effect of more complicated internal structures on the dynamic remagnetization of magneto-polymer composites and biological tissues with the embedded fine magnetic particles.

The proposed method is based on the analysis of the Fokker-Plank equation for the density of probability  $W$  of the dimer particles magnetic moments orientation. Assuming that both dimensionless parameters of the particles dipole-dipole interaction and of the particle magnetic anisotropy are much more than one, we have used modification, for the two particles dynamics, of the mathematically regular Kramers method. The results show that initial susceptibility of a particle in the dimer exceeds the susceptibility of the particle in the single state – this is a consequence of the interparticle magnetic interaction. Because of the dipole-dipole interaction, characteristic time of the dimer remagnetization is much more than the time of remagnetization of the single particle.

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# **Magnetic properties of textured ferrocomposite consisting of immobilized superparamagnetic nanoparticles**

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Wide use of magnetic nanoparticles in modern technologies and biomedical applications requires reliable theoretical models capable of predicting physical properties. Solidification of a ferroparticle suspension under the action of permanent magnetic field allows us to obtain a ferrocomposite, characterized by some orientational texture of the nanoparticle easy magnetization axes. The static magnetic response of this ferrocomposite differs from that of the parent magnetic suspension due to “freezing” of nanoparticle translational and rotational degrees of freedom. Here the superparamagnetic fluctuations of the nanoparticle magnetic moments play a key role in the formation of the ferrocomposite magnetic response depending on the degree of orientational ordering, obtained during synthesis of a ferrocomposite. With the help of statistical mechanics, we calculate the magnetization and the initial magnetic susceptibility of the textured ferrocomposite for various temperatures and magnetic field strengths [1]. The easy axis texturing leads to a significant increase of the magnetic properties, and the effect intensifies with the growth of nanoparticle magnetocrystalline anisotropy. Theoretical predictions are supported by Monte Carlo simulations. The obtained results evidence that the texturing of a ferroparticle suspension and transforming it into a textured ferrocomposite are a real way to enhance the magnetic response of these magnetic soft materials.

The research funding from the Ministry of Science and Higher Education of the Russian Federation (Ural Mathematical Center project, Agreement No. 075-02-2022-877) is gratefully acknowledged.

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# Modeling of the structural and magnetic properties of magnetoactive composites with anisotropic internal architecture: The influence of the interparticle interactions

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This work is devoted to the theoretical study of the structural and magnetic properties of an ensemble of single-domain interacting magnetic nanoparticles immobilized in a non-magnetic medium. This model is typical for describing magnetoactive soft materials – "smart" polymer ferrocomposites, which have been applied in science-intensive industrial and biomedical technologies. It is assumed that the ferrocomposite is obtained by solidification of the carrier medium in a ferrofluid under the external magnetic field, the intensity of which is determined by the Langevin parameter  $\alpha_p$ ; after the solidification of the carrier liquid, the nanoparticles retain the spatial distribution and orientation of their easy magnetization axes.

The features of the orientational texture formed in the sample are analyzed depending on the intensity of the magnetic field  $\alpha_p$  and interparticle dipole-dipole interactions. The magnetization of a textured ferrocomposite in the magnetic field  $\alpha$  is also investigated. Our results show that in the case of a co-directional arrangement of the considered fields and if  $\alpha < \alpha_p$ , ferrocomposites are magnetized much more efficiently than ferrofluids due to their texture. In the fields  $\alpha > \alpha_p$ , the ferrocomposite is magnetized less efficiently than the ferrofluid due to the internal magnetic anisotropy of nanoparticles. The obtained analytical expressions make it possible to predict the magnetization of a ferrocomposite depending on its internal structure and synthesis conditions, which is the theoretical basis for the synthesis of ferrocomposites with a predetermined magnetic response in a given magnetic field.

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