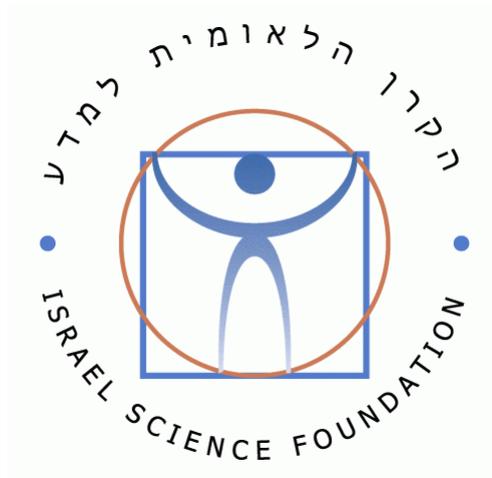


*Tenth International Symposium on*  
**Continuum Models and  
Discrete Systems  
(CMDS10)**

**NATO Advanced Research Workshop  
&  
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**CONFERENCE ABSTRACTS**

# **What controls the rheology of granular materials?**

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I present results from two-dimensional discrete granular dynamics computer simulations investigating the behavior of grain aggregates under different packing densities and boundary conditions. Simulations show a transition between two modes of deformation: solid-like and fluid-like deformations. This “rigidity transition”, which is also confirmed experimentally, has several characteristics of a second-order phase transition. The “phase-boundary” acts as an attractive state for granular systems, where grain aggregates naturally evolve to a state that fluctuates between solid and fluid-like behaviors. A naturally occurring critical state may partially explain the apparent difficulty in formulating a coherent theory for these systems. Analysis of inter-granular contact statistics shows that there exists a large heterogeneity in the forces transmitted at grain contacts, and the distribution of forces on contacts is bi-modal: Contacts that carry large forces (“stress-chains”) are oriented mostly in the maximum compressive direction. Contacts that carry small forces are oriented mostly perpendicular to the stress chains, and play a role in supporting them. Interestingly enough, the weak-force network controls the strength and rheology of the whole aggregate. The structural stability of this weak network is responsible for large-scale instabilities such as stick-slip, and rheological transitions such as the rigidity transition explained above.

## **Analysis of Stochastically Heterogeneous Microbeams by a Functional Perturbation Method**

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Mechanical behavior of heterogeneous beams are important when the beam size is small enough such that morphology is no longer a negligible factor in calculating the macro elastic response (deflections, reaction forces), strength, buckling loads etc. This is the case in MEMS and NEMS technologies, for example when polycrystal structures of micro and nano size are built. In these cases, the use of an equivalent homogeneous structure with the classical effective material properties (RVE) may not be sufficient.

A Functional Perturbation Method (FPM), which has been developed recently to tackle such problems, is described first. The main feature of the method is obtained by treating the global parameters of the structure as functionals of morphological. Then, functional series expansion of the governing equations yields a sequence of ordered equations, which are solved sequentially. For beam problems, the method is basically analytical, and does not suffer from numerical limitations as the Stochastic Finite Element Method (SFEM).

Then, FPM solutions of three types of problems regarding stochastically heterogeneous, linear elastic microbeams will be briefly described: a.) Statistical average and variance of reaction forces and displacements, for which a mechano-statistical reciprocal relation is

found, b.) Strength reliability, based on the weakest link approach, where both elastic and strength properties are random and c.) Buckling loads, including comparison with previously calculated SFEM and Monte Carlo results.

The relation between various morphological properties (grain size, shape, moduli correlations etc) on the overall response will be emphasized. Although Bernoulli assumptions are used throughout, it will be shown that the FPM can be applied to higher order beam models.

## **Power-law coarsening of dislocation froth patterns in two dimensions**

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One of the simplest dislocation models displaying conspicuous pattern formation consists of edge dislocations moving in two dimensions, with glide and climb velocity components (i.e. motion parallel to and perpendicular to the Burgers vector characterizing each dislocation) in linear proportion to the corresponding force components exerted by the dislocations' mutual interaction. This system displays "dislocation cells" (regions almost devoid of dislocations), separated by "dislocation walls" (linear systems of mostly parallel dislocations). When an initially random collection of dislocations belonging to three slip systems (sixfold symmetry) is followed in simulations of this model, the dislocations gradually "anneal out" of the system, and the dislocation cells are observed to coarsen and grow, with their size evolution consistent with a one-third power-law of the elapsed time. This behavior may be contrasted with other models of point-like objects with long-range forces and dissipative dynamics, including systems driven by gravitational or electric fields. An attempt at describing the system at the level of (continuous) dislocation walls, instead of discrete dislocations, will be discussed.

## **Modeling infiltration during soil seal formation: Effects of seal non-uniformity in depth and soil heterogeneity in space**

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The impact of raindrops on the soil surface disturbs the soil upper layer and causes changes in its properties. The result is the sealing of the soil to water infiltration. A dynamic model is developed, that describes soil sealing in terms of the increase of the soil bulk density, being maximal at the soil surface and decreasing exponentially with depth. The formulation of the relationships between the soil bulk density and its hydraulic parameters allows the determination of the hydraulic functions at every point within the disturbed layer and at every moment during seal formation. It is, thus, possible to solve the flow equations not only for the undisturbed soil but also within the seal domain. Once calibrated, the predictive ability of the dynamic model was found to be rather good on basis of verification with extensive experimental results. Therefore, it can be used now to evaluate the effects of various variables affecting flow processes, like soil and rainfall properties, initial conditions, or chemical conditions of the soil-water system, on infiltration and runoff generation.

The dynamic model is used to compare the effects of accounting for the non-uniformity with depth of the seal layer and the areal heterogeneity of the soil hydraulic properties under soil surface sealing conditions on infiltration are studied. The depth dependent properties of the non-uniform seal are expressed in terms of the exponential model of Mualem and Assouline (1989). The dynamics of seal formation are modeled according to Assouline and Mualem (1997). The soil areal heterogeneity is represented by a lognormal distribution of the saturated hydraulic conductivity of the initially undisturbed soil and by related distributions of the other soil parameters.

Accounting for seal non-uniformity has only a minor effect on the infiltration curve during the first rainfall on an undisturbed soil profile, when the seal layer is formed. However, it has a significant effect regarding the dynamic changes of the water content in the soil surface, and consequently, within the seal layer. During subsequent rainfalls on a sealed soil profile, when the seal layer is completely developed, the effect on the infiltration curve is much more significant. Representing the seal as a non-uniform layer decreases the ponding time and the infiltration rates at the early stage of the process. The amplitude of these effects is increased when the rainfall rate is higher and the seal layer is thicker.

Accounting for areal soil heterogeneity reduces the ponding time and the rate of infiltration decrease, while it increases the steady infiltration rate after a long exposure to rainfall. When soil surface sealing is considered, the ponding time is only slightly affected but significantly more runoff is produced. However, the effects of soil variability on the infiltration curve are reduced, compared to the unsealed field. The approximation that the infiltration curve is a unique function of cumulative rainfall independent of rainfall intensity is not valid in a sealing heterogeneous field case. On the other hand, one may disregard the variability of all soil parameters, except the hydraulic conductivity, when calculating infiltration.

## **THE SPECIAL ELECTRICAL PROPERTIES AND THE CORRESPONDING APPLICATIONS OF CARBON BLACK-POLYMER COMPOSITES**

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The electrical properties of carbon black-polymer composites are of great interest from both, the basic physics and the commercial-applications points of view. Correspondingly, these

properties have been studied intensively in the last thirty years (1). Starting from the physical understanding, one notes that as a binary system composed of a conductive phase, made of carbon-black (CB) particles, and an insulating phase, made of a polymer, the system is widely considered as a prototype of a “metal-insulator” composite. The electronic properties of the CB-polymer composites were explained then for many years within the framework of inter-particle tunneling conduction (2) on the one hand, and as a percolation network of the corresponding conductances (3) on the other hand. However, these two basic pictures for the understanding of the system are not conceptually compatible with each other, and their combination does not provide an explanation for the many contradicting experimental data. The incompatibility follows the facts that, in contrast with the conventional percolation model, in this system, no two particles are connected geometrically (as, say, in granular metals above the percolation threshold), but any two conducting particles are connected electrically by tunneling conduction (4). A conspicuous example of the contradictions in the experimental results is the verity of results obtained when a percolation approach is applied for the analysis of the data. The analysis reveals strong dependencies of both; the (apparent) percolation threshold,  $x_c$  (where  $x$  is the volume % of the CB in the composite and  $x_c$  is its critical value) and the (apparent, see below) percolation critical exponent  $t$ , on the particular type of the CB used in the composite (5). The explanation of these results with a “unified model” constitutes then an exciting challenge.

From the industrial-technical point of view we note that the present system has been proven to yield many mechanical and electrical applications (6), notably, the billion-dollar market of overcurrent protection and current self-regulating devices (7). While the original reason that yields this property (i.e. the Positive Thermal-expansion Coefficient-PTC of the polymer) is well known, there is still a wide and intensive debate as to the manifestation of this effect in the observed behavior (8).

Following the above considerations we have carried out an extensive experimental and theoretical study in order to obtain a comprehensive understanding of the electrical transport in the CB-polymer composites (9). Very recently we have extended our study to include the local aspects of the electrical properties of the system by applying the Contact resistance Atomic Force Microscopy (C-AFM) technique (10). As will be discussed at the workshop, we have been able to determine the reason for the global percolation-like properties of the system and to find the details of the electrically induced switching effect. In particular we found that the global phenomenon is due to many independent switching and reconnection events.

Acknowledgement: This work was supported by the Israel Science Foundation.

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## **A fractal model for the sea state bias in radar altimetry**

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The Kirchhoff approximation is used to determine the sea state bias in radar altimetry. A weakly nonlinear model of the sea waves is used to derive the joint moments of two different points separated by a distance  $R$ . The bias moment is formulated and found for power low spectra. The method provides a consistent analysis of the sea state bias and avoids the need to truncate the high frequency tail of power-low wave spectra. The model exhibits dependence of the "electromagnetic bias" on the radar frequency, an effect observed in field experiments.

## **Noise in Non-Ohmic regimes of Disordered Systems**

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Disordered systems in general are driven into nonohmic regimes under a sufficiently large bias. Resistivity either decreases or increases depending upon the transport mechanism that comes into play. The nonohmicity leads to current redistribution which is expected to have strong effect on the associated noise. It is found that the noise does not simply follow the resistance. It does vary as the resistance but is controlled by parameters different from those responsible for the onset of nonohmicity. Such property makes the noise an important tool for studying complex systems such as disordered ones, specially in the nonohmic regimes. There are also other unique properties in time and frequency domains. An attempt will be made to review these properties in relation with those in the ohmic regimes.

# **Diffusion equation with fractional time derivative – physical sense and practical realization**

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Diffusion equation with fractional time derivative is analyzed in a framework of the continuous random walk model (CTRW). Whereas the CTRW model has the clear advantage of being based directly on physically motivated random walk schemes, the fractional equation is often introduced *ad hoc* and is thus of a phenomenological character. Moreover the “games” with fractional derivatives result to loss the physical sense of any Fokker-Plank equation as a continuity equation in suitable space.

It is shown that the equation acquires physical sense if some real “drain” term is incorporated in the equation. The equation governs the space-time evolution of a packet of delocalized particles propagating across a sample with some special traps. The number of particles does not conserve through the trapping. The “drain” term describes the net effect of these traps on the total number of the delocalized particles.

The exact form of this term is unknown *a priori*. It is possible only to find the relation between the to rate of decreasing of the total number of the delocalized particles and the divergence of mean trapping time.

The real physical situations suitable of the model are discussed. The simple diffusive substrate compatible with CTRW model, so-called comb-structure is investigated in details both theoretically and experimentally. The concrete form of the drain term is found. It is shown that the space-time evolution of a packet of delocalized particles is described by standard integro-differential continuity equation of CTRW model with drain term proportional to rate of decreasing of the total number of the delocalized particles.

## **Continuum field model of defect-induced heterogeneities in a strained thin layer**

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Recently, it was argued that electrical and magnetic properties of a surprisingly great amount of perspective materials are very sensitive to (apparently weak) sample imperfections [1]. In particular, colossal magnetoresistance manganites that exhibit multiphase coexistence are characterized not by enhanced linear response to disorder but by a low threshold to a qualitatively different nonlinear response. In this contribution, I report similar mechanical behavior in strained damage layers of cobalt disilicide and stabilized zirconia and present a theoretical analysis aimed to explain the nucleation of inhomogeneous regions in the layers under a uniaxial stress.

Our continuum model describing the effect of elastic stresses on an amorphous solid with extending defects is based on the introduction of an order parameter field of distributed defects (vacancies and interstitial impurities) coupled with a displacement field. We consider the one-dimensional geometry focusing, in particular, on the phenomenology of a first-order transformation in the inhomogeneous elastic medium with different volumes of product and parent phases. The phase-field equations minimizing the total free-energy functional incorporate the physics of the defect subsystem and the macroscopic behavior of a strained solid that follows from the conventional theory of elasticity. Numerical simulations show that (i) the interaction of two phase fields results in their inhomogeneous redistribution along the sample; (ii) this factor can reduce a threshold, above which the material properties change dramatically. The concept of inhomogeneity is applied to explain the roughness of a cobalt disilicide layer grown on a silicon surface by a conventional silicidation procedure [2] as well as our three-point bend-test experiments on stabilized zirconia samples undergoing the martensitic transformation. The data for stress-induced transformation toughened zirconia provide novel arguments supporting the idea about defect-triggered nucleation of a martensite in a crystal [3].

This work has been done with experimental groups from the Donetsk Physical and Technical Institute, Donetsk, Ukraine (G.Akimov and Yu.Komysa), Institute for Metal Physics, Kiev, Ukraine (I.Belousov), and Friedrich-Schiller-Universität, Jena, Germany (P.Seidel).

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## **Bio-Inspired Engineered Self-Organization**

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The rapid developments in communication, informatics and nano- and bio-technologies give rise to a new difficulty: how to build a complex functioning system from a large number (say,  $10^{10}$ - $10^{12}$ ) of smart, man-made interacting elements. Such systems are too complex for design and for blueprint construction. The challenge is to develop a new engineering methodology for the creation of such systems.

Currently, despite the great progress in computational power, we have not reached even the ability to simulate the intracellular gel of a single bacterium, the simplest living organism, let alone design one. This macromolecular plexus, composed of  $\sim 10^{11}$  interacting polymers, proteins and nucleic acid segments, each with its own internal structure, continuously re-organizes its structure and composition in response to external stimuli and according to information stored in the DNA. Nature has not built such gels, cells, organs and organisms following some pre-designed blueprint, but rather via a process of biotic self-organization.

I have conducted in parallel investigations of bacterial and neuronal self-organization, seeking to unravel the general principles of biotic self-organization. This

endeavor proved successful, and our level of understanding is now such that I feel it can hint at a new approach to building complex man-made systems.

Our central nervous system is composed of  $10^{11}$ - $10^{12}$  neurons with about  $10^{16}$  synaptic connections. A typical bacterial colony consists of  $10^9$ - $10^{12}$  bacteria. Both systems are not created by pre-design or according to a plan, but through a process of biotic self-organization. The elements (neurons or bacteria) do not store the information required to construct the system, but rather the information for creating the needed “tools” and the guiding principles. Additional information is cooperatively generated as the organization proceeds following external stimulation. The key principles that enable it are communication and self-plasticity of the components. The outcome is an adaptable complex system that can perform many tasks, learn and change itself accordingly. Consequently, the idea of engineered self-organization is to let many collections of element self-organize in a pre-engineered environment they can exchange information with. The most efficient collections will be let to further self-improve via genetic algorithms of the components internal structure and capabilities (the analog of evolution of the potential for gene expression). The system itself should regulate the evolution of its components.

I'll conclude with projections in regards to turning the conceptual idea, of engineered self-organization of communicating elements with self-plasticity, into an operational approach that will enable the creation systems too complex for design, yet with desired pre-specified capabilities.

## **Exact relations between critical exponents for elastic stiffness and electrical conductivity of percolating networks**

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It has long been known that the critical exponent  $T$  of the elastic stiffness  $C_e \propto \Delta p^T$  of a  $d$ -dimensional percolating network ( $\Delta p \equiv p - p_c > 0$  measures the closeness of the network to its percolation threshold  $p_c$ ) satisfies the following inequalities  $1 + d\nu \leq T \leq t + 2\nu$ , where  $t$  is the critical exponent of the electrical conductivity  $\sigma \propto \Delta p^t$  of the same network and  $\nu$  is the critical exponent of the percolation correlation length  $\xi \propto |\Delta p|^{-\nu}$ . Similarly, the critical exponents which characterize the divergences  $C_e \propto |\Delta p|^{-S}$ ,  $\sigma_e \propto |\Delta p|^{-s}$  of a percolating rigid/normal network (i.e., a random mixture of normal elastic bonds and totally rigid bonds) and a percolating superconducting/normal network (i.e., a random mixture of normal conducting bonds and perfectly conducting bonds;  $\Delta p \equiv p - p_c < 0$  now measures the closeness of the rigid or superconducting constituent to its percolation threshold  $p_c$ ) have long been known to satisfy  $S \leq s$ . I now show that, when  $d=2$  or  $d=3$ ,  $T$  is in fact exactly equal to  $t + 2\nu$  and  $S$  is exactly equal to  $s$ . This is achieved by a judicious use of some variational principles for electrical and elastic networks, and by a

judicious treatment of constraints and short range correlations in those networks. The detailed proofs appear in Refs. [1,2]. They rely on an important assumption, namely, that the critical behavior of the macroscopic conductivity of a percolating three-constituent network of bonds with three very widely differing (i.e., by orders of magnitude) bond conductances is the same as that of the more usual two-constituent percolating networks. This assumption has been tested by numerical simulations of random networks, as reported by Xiangting Li in the poster session of this workshop [3]. An extension of the above mentioned proofs to arbitrary (integer) values of the dimensionality  $d$  should also be possible.

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## **Discrete Network Approximation for Effective Properties of High Contrast, Random, Highly Packed Solid and Fluid composites**

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We present a new approach for calculation of effective properties of high contrast random composites (random particles in a matrix or host when properties of the particles and the hosting medium are very different) and provide its rigorous mathematical justification. The main idea of this approach is the reduction of the original continuum problem, which is described by PDE with rough coefficients, to a discrete random network. We introduce the inter-particle distance parameter for irregular (non-periodic or random) distributions of particles and show asymptotic equivalence of the effective (homogenized) coefficients for the discrete and continuum models in the limit when the relative interparticle distance goes to zero. Our method is based on variational techniques and it provides an exact error estimate in which all constants are explicitly defined. Such results are rare in homogenization: most of the error estimates provide the order of magnitude only and involve some unknown constants. Our study was motivated by a problem of optimizing effective properties of polymer/ceramic composites and coal/water slurries. We use the discrete network to compute the effective coefficients (effective dielectric constant, effective viscosity) numerically and draw physical predictions about poly-dispersed composites (particles of different sizes) in the percolation regime. The work was done jointly with A. Kolpakov [1], with A. Novikov [2], and with L. Borcea and A. Panchenko [3].

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## **Damage mechanisms and fracture of glass at the nanometer scale**

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The morphology of fracture surfaces of glass and metallic alloys have been shown to exhibit amazing similarities, but at very different scales of observation. Both kinds of surfaces present two self-affine regimes. At small length scales/low average crack velocities, they are characterized by a roughness exponent close to 0.5. At larger length scales/higher average crack speeds, this exponent is close to 0.8. Although the values of these exponents do not vary with the material, the range of length scales where these regimes appear is very sensitive to its structure. In the case of glass, the 0.5 regime extends up to ~10nm while the 0.8 regime extends up to some 100 nm. In the case of some metallic alloys, the first regime may extend from 5nm to 30 $\mu$ m, and the second one up to 0.5mm. Is this similarity in fracture surfaces morphologies at different length scales due to a similarity in the damage and crack propagation mechanisms?

The presence of damage cavities ahead of the crack tip in glass, actually predicted by Molecular Dynamics Simulations, could also explain the departure from linear elasticity observed in the vicinity (~50nm) of a stress corrosion propagating crack in glass.

Our *in situ* Atomic Force Microscopy experiments clearly show the existence of such nanometric damage cavities, i.e. that *glass breaks like metals, but at the nanometer scale*. The width of the damage cavities is indeed of the order of magnitude of the crossover length separating the two self-affine regimes. We also show that they are at the origin of the departure from linear elasticity, observed in the damaged zone.

A model based on the emission of crack front waves propagating along the extending border of the growing cavity is shown to predict the small length scales roughness exponent (0.5). The orders of magnitude are in fair agreement with the observations.

# **Dynamic Critical Phenomena in Plastic Deformation, Failure and Fatigue in Random Fiber Bundle Model**

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Dynamics of failure in random fiber bundle model, where the fiber strengths are given by simple distribution functions and where the load on the bundle is shared globally by all the intact fibers uniformly, are studied analytically. Dynamic and static critical exponents for fracture breaking are all obtained (in this mean field limit). Exact results for plasticity in these models are also derived and the breakdown avalanche etc. results are compared with numerical results. Fatigue behaviour in such models are also studied approximately in presence of noise and compared with the numerical results.

## **Elasto-plastic models of crystalline materials with continuous distribution of dislocations based on the configuration with torsion**

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In the present paper we propose models of crystalline materials with continuous distribution of dislocations, based on the concept of configuration with torsion. The irreversible part of the deformation gradient is defined in terms of the configuration with torsion. The existence of the dislocations can be identified at the macroscopic level through the different measure of the inhomogeneities, such as: plastic torsion, plastic cotorsion or curl of the plastic part of deformation. Just the second order gradient associated with the configuration with torsion gives rise to the plastic inhomogeneities, via the plastic connection. Based on the definitions inferred in the model the multiplicative decomposition of the deformation gradient follows, the appropriate relationships between the elastic, plastic and motion connection, as well as between their rates, are derived. The models are developed within the constitutive framework proposed in Cleja-Tigoiu, ZAMP, 53, 2002, 996-1013. The energetic arguments in choosing the set of variables and the coupling between the elastic and plastic properties are delivered by the kinetic energy

theorem. The constitutive equations proposed in the paper describe the behavior of the material with respect to the configuration with torsion, in terms of the symmetric part of Cauchy stress and the third order tensor of stress momentum. The evolution equations for the configuration with torsion as well as for the plastic connection are introduced to close the theory. We emphasize the role of the connection with torsion in the describing the behavior of the material and the differences between our models and the Cosserat type theory for elastoviscoplastic crystalline materials at finite deformations developed for instance in Forest, Cailletaud, Sievert, Arch. Mech. 49, 1997, 705-736.

Theory of a naturally discrete model for DNA elasticity that accounts for the dependence of the mechanical properties of DNA on nucleotide sequence.

## **Clausius-Mossotti-type approximation for elastic moduli of a cubic array of spheres**

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The method of elastostatic resonances [1] is applied to the 3D problem of non-overlapping spherical inclusions arranged in a cubic array in order to calculate the effective elastic moduli. The approach is based on an expansion of the strained state of the composite material in terms of elastostatic resonances (eigenstates): These are (unphysical) states where the sample is internally deformed and strained even though its boundaries are undeformed. The approximation used, which is the leading order in a systematic perturbation expansion of the appropriate elastic modulus, is related to the Clausius-Mossotti (CM) approximation of electrostatics. It takes into account the dipole-dipole interaction between strain fields of different inclusions.

Using this approximation, explicit simple algebraic expressions, exact at least to order  $p^3$  (where  $p$  is the volume fraction of the inclusions), are obtained for the bulk modulus and for the two shear moduli [2]. Some of the expressions turn out to be identical to the Hashin-Shtrikman bounds.

Comparison with numerical calculations and with previous work reveal that this approximation provides accurate results at low volume fractions and is a good estimate at moderate volume fraction even when the contrast is high. This indicates that the CM-type approximations are exact up to orders of volume fractions which are higher than  $p^3$ , in analogy with the 2D problem of a square lattice of cylindrical inclusions [1], where it was found that the corrections to the CM-type approximations begin with order  $p^5$  for the bulk modulus, and with order  $p^4$  for the shear moduli.

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# **Theory of a naturally discrete model for DNA elasticity that accounts for the dependence of the mechanical properties of DNA on nucleotide sequence**

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Although there are cases in which one can treat a (duplex) DNA molecule as an idealized elastic rod that is inextensible, intrinsically straight, transversely isotropic, and homogeneous, it is known that the genetic information in DNA determines not only the amino acid sequences of encoded proteins and RNA but also the geometry and deformability of DNA at a local level, i.e., at the level of nucleotide base-pair steps. Recent advances in structural biochemistry have provided evidence that not only the geometric properties but also the elastic moduli of duplex DNA are strongly dependent on nucleotide sequence and exhibit features that are not accounted for by classical rod models of the Kirchhoff type.

In recent joint research, David Swigon, Wilma Olson, and the speaker [1] have formulated a theory of a general class of models in which the contribution of the  $n$ -th base-pair step to the elastic energy of a DNA molecule is taken to be a function  $\tilde{\psi}^n$  of six kinematical variables that describe the relative orientation and displacement of the  $n$ -th and  $(n + 1)$ -th base pairs; these variables are called tilt, roll, twist, shift, slide, and rise. Such models can be said to be "naturally discrete"; for, when they are regarded as discretizations of a continuum, the distance between discretization points (approximately 3.4 Angstroms) has the physical interpretation of distance between the barycenters of successive (domino shaped) base pairs, and the stress-free values of the kinematical variables and also the functions  $\tilde{\psi}^n$  vary greatly from one discretization point to another.

In the paper cited below, one will find symmetry relations imposed on the functions  $\tilde{\psi}^n$  by the complementarity of nucleotide bases (i.e., of A to T and of C to G), the antiparallel alignment of DNA strands, and the requirement that the functions  $\tilde{\psi}^n$  be invariant under change in the direction of increasing  $n$ . In that paper we derive variational equations of equilibrium and present an efficient method for solving those equations and determining the stability of computed solutions when the functions  $\tilde{\psi}^n$  are quadratic forms. To illustrate applications of the theory, we have employed the method to calculate configurations and elastic energies for 150 base-pair DNA minicircles made up of two types of base-pair steps arranged in such a way that each molecule has a nearly circular stress-free configuration and hence can be called a (closed) DNA o-ring. To obtain information about the effects of bound ligands on DNA configurations one can impose local untwisting of variable magnitude at selected base-pair steps. We have found several cases in which the response of DNA o-rings to such untwisting is markedly different from that of minicircles of intrinsically straight DNA. A study has been made of the influence on equilibrium configurations of cross-terms in the functions  $\tilde{\psi}^n$  that couple twisting to bending (i.e., twist to roll).

Recent research of Yoav Biton, done in collaboration with David Swigon and the speaker, has yielded a method of calculating the influence of electrostatic forces on equilibrium configurations of intrinsically curved DNA obeying the present theory of sequence-dependent elasticity. Among his results to be presented at the Symposium are calculations showing how the minimum energy configuration of a highly curved DNA molecule of helical shape extends and straightens out as the concentration of monovalent salt is decreased from 1 molar to  $5 \times 10^{-6}$  molar.

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## **PHENOMENON OF "DISCRETE" ("QUANTIZED") OSCILLATION EXCITATION**

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A phenomenon of "discrete" ("quantized") oscillation excitation has been found and studied both numerically and analytically. Multiple bifurcation diagram for the attractor set of the system under consideration has been obtained and analyzed. The complex dynamics, evolution and the fractal boundaries of the multiple attractor basins in state space corresponding to energy and phase have been obtained, traced and discussed. A two-dimensional discrete map has been derived for this case. A general treatment of the class of kick-excited self-adaptive dynamical systems has been made by putting it in correspondence to a general class of discrete dissipative twist maps and showing that the latter is an immanent tool for general description of its behavior.

The class of kick-excited self-adaptive dynamical systems that has been formed and proposed is characterized by a nonlinear (inhomogeneous) external periodic excitation (as regards the coordinates of the excited system) and is remarkable for the occurrence of the following objective regularities: the phenomenon of "discrete" ("quantized") oscillation excitation in macro-dynamical systems having multiple branch attractors and strong self-adaptive stability. The main features of the class of systems are studied on the basis of the general model of a pendulum under inhomogeneous action of a periodic force (referred to as a kicked pendulum). An analytic proof is presented showing the existence of discrete ("quantized") oscillations for the kick-excited pendulum. Generalized conditions for the excitation of pendulum oscillations (with a discrete set of possible stationary amplitudes) under the influence of an external non-linear force are derived.

A generalized model of an oscillator, subjected to the influence of an external wave is considered. It is shown that the systems of diverse physical background which this model encompasses by their nature should belong to the broader class mentioned of "kick-excited self-adaptive dynamical systems". The theoretical treatment includes an analytic approach to the conditions for emergence of small and large amplitudes, i.e. weak and strong non-linearity of the system. Derived also are generalized conditions for the transition of

systems of this "oscillator-wave" type to non-regular and chaotic behavior. For the purpose of demonstrating the heuristic properties of the generalized "oscillator-wave" model from this point of view are considered the relevant systems like kick-rotator and phenomena of the quantized cyclotron resonance and the mega-quantum resonance-wave model of the Solar System. We point to a number of other natural and scientific phenomena which can be effectively analyzed from the point of view of the developed approach. In particular, we stress on the possibility for development and the wide applicability of specific wave influences, for example for the improvement and the speeding up of different technological processes. A wide spectrum of applications of the formed class of systems is presented.

## **LYAPUNOV EXPONENTS AND STABILITY AND BIFURCATIONS OF CHAOTIC ATTRACTOR IN COUPLED TENT AND LOGISTIC MAPS**

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At present time a study of endomorphisms of the plane  $R^2$  constituted by coupling of two identical endomorphisms of the line  $R^1$  becomes a matter of steady topical interest. At that rather often one consider so-called "coupled tent maps" or "coupled logistic ones". Researching them with aid of computer numerically and, in particular, calculating their Lyapunov exponents physicists found conditions of stability as well as bifurcation of their non-trivial "diagonal" attractors and stated that *i*) the attractors are asymptotically stable in  $R^2$  if they are asymptotically stable as subsets of  $R^1$  and their "transversal Lyapunov exponents" (calculating in the attractor points) all are negative; *ii*) a loss with the attractor of asymptotic stability and start of process of bifurcation of the phase pattern in the attractor vicinity has with origin an appearance of positive "transversal Lyapunov exponent" at a fixed or periodic point embedded the attractor. But since any computer makes calculations with certain precision and therefore nobody can absolutely exactly know values of quantities one calculate, hence still is a question on how these results are related with studying phenomenon. In the report we intend to present a series of rigorously proved mathematical results concerning properties of the maps mentioned above. In particular, we point out parameters values such that the coupled tent (logistic) maps have the non-trivial diagonal attractor and, moreover, we find that its asymptotic stability and bifurcation are completely conditioned on values of the map transversal Lyapunov exponent at the fixed point embedded the attractor.

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## **The Micro-Branching Instability and the Dynamic Fracture of Brittle Materials**

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We review recent experiments performed on PMMA (poly-methyl-methacrylate) and glass. The results of these experiments offer a new view of the dynamic fracture process. We will show that the transition from a state consisting of a single propagating crack to a multiple crack state is the result of a *dynamic instability*. This instability appears as the velocity of the crack exceeds a critical velocity,  $v_c$ . Below  $v_c$  a single crack is observed, the crack velocity is a smooth function of time (increasing or constant, depending on experimental conditions) and the fracture surface created is smooth and mirror-like. Beyond  $v_c$ , a single crack state no longer exists. Instead, small microscopic side branches will bifurcate from the crack (micro-branches) whose dynamics are inter-related with those of the main crack. As a function of the mean velocity of the crack,  $v$ , these branches increase in length as the mean dynamics of a crack change dramatically; the crack velocity develops oscillations, and non-trivial structure is formed on the fracture surface. Both the amplitude of the oscillations in the crack velocity and the amplitude of the structure formed on the fracture surface increase with the length of the micro-branches found below the fracture surface. As the branches grow in size, they evolve into macroscopic, large-scale crack branches. Thus, the instability provides the crucial link between a single crack state, at low energy flux (low velocities) and the multi-crack states, which include both micro-crack states and macroscopic branching, at high energy fluxes.

Below  $v_c$ , we will show that the dynamics of the single-crack state is in excellent quantitative agreement with theoretical predictions. Above  $v_c$ , quantitative measurement of both the energy flux into the tip of a moving crack reveals that the micro-branching instability is the main mechanism in these materials for the increase in the dissipation of energy (i.e. the fracture energy) by a moving crack at high velocities. In these materials the

rate of new surface creation, beyond  $v_c$ , is proportional to the energy flux into the tip of the crack, and the micro-branches possess a characteristic form. This mechanism provides a simple explanation for both the observed velocity dependence of the fracture energy and for the question of why the limiting velocity of a crack, the Rayleigh wave speed, is never realized. This scenario provides a simple picture of how a single fracture event can create the highly ramified structures that are often observed.

## **Spin Effects in Plasticity**

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A magnetic field may influence dynamics of dislocations. A moving kink of a dislocation, when passing a paramagnetic obstacle, may form a radical pair in a singlet or triplet spin states, one of which is binding, whereas the other one is antibinding. Magnetic field induced intercombination transitions between the binding and antibinding states may influence dislocation detachment from the obstacles, and in particular enhance the detachment probability. This microscopic mechanism allows one to explain various experimental observations, among which: magnetic field dependence of the internal friction, electroplastic and magnetoplastic effects, resonance enhancement of dislocation mobility under the influence of a microwave magnetic field, isotope effect, and other. In ferromagnets the role of the magnetic field is taken by the fluctuating local spontaneous magnetization. It is shown that the dislocation mobility should critically increase near the Curie point.

## **Geometrical factors affecting the bulk electrical properties of soils and rocks: Measurements and continuum mean field computations**

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Understanding the relationship between the effective electrical conductivity and dielectric permittivity of soils and rocks and their porosity and volumetric water content is important because measurements of electrical properties are used to determine porosity and water content. In this lecture we are going to report experimental and theoretical studies aimed at improving our understanding of the way the geometrical attributes of granular materials determine their effective conductivity and permittivity [2-5]. In order to avoid interfacial surface conductivity and bound water effects we have used coarse granular materials of low surface area such as glass beads, quartz sand grains, tuff and mica particles. Accurate measurements of the effective electrical conductivity [4,5] and permittivity [2-5] of anisotropic packings of mica particles [2] and isotropic packings of glass beads, sand

grains and tuff particles [3-5] have demonstrated: 1, an alteration of the directional effective conductivities and permittivities of anisotropic packings attributed to particle shape and orientation; 2, a reduction in the permittivity of isotropic packings due to deviation from a spherical particle shape and an increased broadness of particle size distribution. The measured effective conductivities and permittivities are predicted reasonably well by modified classical mixing formulas [2-4], reviewed in e.g. [1]. Particle shape effects were modeled using the depolarization factors of equivalent oblate particles [2,4] and those of particle size distribution using a finite number of inclusion-intermediate background mixing [3]. For dense granular packings of various particle shapes and size fractions, of a background/inclusion conductivity ratio of 1/8 to 80 the effects of the neighboring particles can be accounted for with a single value,  $a = 0.2$ , of a heuristic parameter  $a$  defined in the range of 0 (Maxwell/Clausius-Mossotti mixing law) to 1 (coherent potential approximation).

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## **MODELING OF CHAIN MOBILITY IN LOADED AN ORIENTED CRYSTALLINE POLYMER**

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In the model interconnection molecular chains in an oriented linear crystalline polymer were fastened on or near polymer crystallite surface by intermolecular bonds or cross-links. Simple cosine periodic potential as in Frenkel-Kontorova's dislocation model was used for intermolecular interaction and condition of balance of loaded chain in polymer crystallite.

The dislocation formation is accompanied molecular chains slippage and local loads relaxation on their amorphous sections as well as by conformation regroupings of these sections in some conditions. In dependence on external load and amorphous region length different cases are realized. The first case takes place when the load is moderate. In this case the load on the amorphous section of a slipped out chain are completely relaxed and this section could change its conformation state. In the another case slipped out amorphous section of a macromolecule is in strained state but its strain is less than one of the macromolecule before its slipping out.

The load relaxation value influences on dislocation behaviour. This behaviour depends except for of macromolecular chain parameters mainly from sizes of stressed amorphous section and of initial load on it. If after dislocation formation this amorphous section remains enough stressed, the dislocation remains in crystallite. In other cases the chain pulled into crystallite again with restoration of load value on amorphous section.

The dislocation movement into crystallite and accordingly the further slippage of the passage macromolecule fastened by cross-link happens with increase of local load on crystallite boundary and with enhance of dislocation energy. While for the passage macromolecules without cross- linking the slippage is accompanied by loss of the energy.

## **Information theoretical sliding window optimization applied to discretization of continuous signals**

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Sliding window analysis is common to many time domain signal analysis methods. Determination of the optimal window width requires several different conditions to be met. Intuition into the signal or knowledge of limitations of computational resources could help; or an optimization scheme may be carried out. Balance between information loss and computational complexity must be met in any case. In a recent study, the authors proposed an optimal windowing method through minimization of the average mutual information between sliding windows. It was meant to determine the optimal input layer width of an artificial neural network to extrapolate time domain data from electromagnetic simulations. They extended it to an optimal sampling scheme. In the one step limit, discretization of continuous signals is another kind of windowing. A continuous signal sampled with infinite-frequency, -which is the signal itself- has the maximum average mutual information between sliding windows. This can be interpreted as waste of resources. Decreasing the sampling rate generally results in a nonlinear decay of the average mutual information between windows. The first minimum, at which the decay settles down before increasing again, generally corresponds to the optimal sampling rate.

# **Force Chains, Microelasticity, and Macroelasticity**

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Some recent experiments and theories suggest that (near) static granular and nanoscale materials exhibit departures from elastic behavior even at infinitesimal loadings. It is demonstrated, through a study of the forces and stress fields in finite discrete systems, that (at least some of) the pertinent phenomena (force chains, properties of Green's functions) are consistent with elasticity (at times even with isotropic elasticity), although the small scale behavior of discrete elastic systems may be different from the bulk behavior, a crossover occurring as the system size is sufficiently large (typically of the order of 100 interparticle distances). Interestingly, frictional forces among the grain may promote elastic behavior by decreasing the degree of rearrangement result from the application of external forces. Some of the features, which may suggest an apparent non-elastic behavior, can be attributed to finite size effects, anisotropy and boundary conditions. Some of the above results, though nominally obtained for models of granular systems, should be relevant to nanometric systems as well.

## **ENERGY AND SYMMETRY OF SELF-ASSEMBLED 2D DIPOLE CLUSTERS**

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We report on 2D dipole clusters formed by small ferromagnetic particles floating at the liquid-air interface and confined within an almost parabolic potential provided by the nonhomogeneous external magnetic field. The particles self-assemble into hexagonally-ordered clusters whose size and lattice constant can be magnetically tuned. We study experimentally the energy  $E$ , the chemical potential, and the lattice constant of 2D clusters as a function of particle number. We develop a continuum model (similar to Thomas-Fermi model for atoms) which accounts fairly well for the smooth part of the  $E(N)$  dependences. However, on top of this smooth dependence we observe quasiperiodic fluctuations with dips at "magic" numbers corresponding to particularly symmetric particle configurations. We demonstrate experimentally and theoretically that these fluctuations are related to the cluster symmetry and to the center of mass position, as predicted by A.A. Koulakov, B.I. Shklovskii, [Phys. Rev. B 57, 2352 (1998)].

# **Transport properties of densely packed fluid/solid and solid/solid composites: Effect of shapes and spacings of inclusions**

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We present an analysis of transport properties of composite structures containing closely spaced rigid inclusions. The host medium may be either an elastic matrix or an incompressible fluid. We use a unified framework based on asymptotic expansions in terms of inter-inclusion distances in order to obtain optimal geometric configurations of finite arrays of inclusions imbedded into the medium. We compare the effective transport properties of the composite material containing inclusions with either flat or curved boundaries. Furthermore, for various applied loads and shapes of inclusions, we show that the "optimal" configurations may involve non-uniform distribution of inclusions of different sizes.

## **TRANSFORMING TO CHAOS USING NORMAL FORMS**

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It is an attractive idea to replace a system by a locally equivalent, simpler system and a polynomial transformation. It is hoped that such a decomposition would approximate chaos by stretching and folding the solution to this simpler system with the polynomial transformation. The method of normal forms achieves this end by a systematic procedure. If there are no resonances, the simpler system is linear, if there are resonances, the resulting system possesses nonlinear terms, but its truncations can often be integrated. Such approaches have been used to study bifurcation schemes locally. We seek to investigate the possibility of extending the normal form approach to the nonlocal task of qualitatively estimating Lyapunov exponents and attractor sizes. Our investigations have revealed both successful and unsuccessful instances of such an estimate.

It is well known that chaotic behavior sets in when at least one of the eigenvalues of the linearized system is positive and the eigenvalues pass from the Poincaré domain to the Siegel domain. For this purpose, a number of chaotic systems with three degrees of freedom and quadratic nonlinearities that have been proposed by Sprott have been studied. Since the Sprott systems do not have any free parameters, it is essential that these systems be generalized in such a way as to introduce a parameter which causes the bifurcation to a positive eigenvalue and transition from the Poincaré to the Siegel domain. Additionally, a has been studied.

A parallel question is studying whether truncations to resonant systems that one obtains with the normal form expansion possess Lyapunov spectra that are comparable with those of the original one. This question requires one to study different algorithms that generate augmented systems of ordinary differential equations (Wolf-Benettin, Wiesel, Ruelle-Eckmann) and numerical integration schemes (Runge-Kutta, Adams-Bashford Bulirsch-Stoer algorithms, direct series expansion and Chebyshev economization). The aim is to find an optimal approach, for numerically investigating generalized versions of certain Sprott systems and the nuclear spin system proposed by Khomeriki.

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# **Dispersive durable systems: The technology of synthesis with given properties.**

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The class of composite materials durable dispersive with firm inclusions and consequently shown with discrete systems are offered for discussion. The index characterizing organization of these systems is developed. The criteria diagnosing structural condition of dispersive durable composite materials (DDCM) – models of discrete systems – are offered. The technology of designing component of DDCM and the technique of their synthesis with the given properties are recommended for practical use. The results of researches are offered according to the value of influence of construction of DDCM on operational indexes armed with products by them. The mathematical models of products armed with DDCM as the differential equations and scalar models in space of conditions are developed. The regime wearing process of armament from DDCM are classified and the algorithm of management by these regimes is developed.

## **RESTRUCTURING OF FORCE NETWORKS**

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The compaction of granular packings or soils is a collective process which for higher densities becomes increasingly slower reaching glassy behaviour. We will look at this problem from various points of view, in particular we will represent the evolving force network that percolates through the system by an inverse fiber rupture model. We will also discuss the case where the sizes of particles are distributed according to a power law, which gives hierarchical compaction dynamics.

# **Integral representation for the solution of some nonclassical one-dimensional pseudoparabolic problems**

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A linear multipoint problem is investigated for some classes of higher order pseudoparabolic equations with generally nonsmooth coefficients. A new concept of the adjoint problem defined as a system of definite integral equations is introduced for this problem. An extension of the superposition principle is obtained by a concept of a fundamental solution which is introduced as a particular solution of the corresponding adjoint system of the integral equations. Such a fundamental solution exists under some conditions like as  $p$ -integrability and boundedness on the coefficients. This fundamental solution can also be considered as a natural generalization of the classical Riemann function concept for nonlocal problems and nonsmooth coefficients.

## **Representative Volume Element: a statistical point of view**

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The Representative Volume Element (RVE) plays a central role in the mechanics and physics of random heterogeneous materials with a view to predicting their effective properties; however, its definition is usually unclear. In this presentation, we propose a statistical approach of this notion, where a quantitative definition of the size of the RVE can be proposed. Starting from realizations of a random medium in a finite domain  $D$ , estimations of the effective properties are given by averaging the field properties (for instance the stress and strain in elasticity) over  $D$ . Fluctuations of the fields, and of the estimated averages result from the randomness of the medium, and from the finite size of  $D$ . Using the variance of the averages as a function of the volume  $V$  of  $D$ , a RVE size can follow from the choice of a given precision of the estimation of the wanted overall property. It is shown to depend on the investigated morphological or physical property, the contrast in the properties of the constituents, and their volume fractions. The bias introduced by the choice of specific boundary conditions prescribed to each domain  $D$  is also discussed in detail, regarding three main types of boundary conditions: strain-based or

stress-based homogeneous boundary conditions, on the one hand, and periodicity constraints, on the other hand. The methodology is applied to a specific model of random microstructure, namely a two-phase three-dimensional Voronoï mosaïc, and to a real microstructure studied in 3D by means of confocal microscopy. Solutions of the linear elasticity and of the heat conduction problems are obtained by finite element calculations on increasing volumes. They enable us to provide estimates of the key notion of integral range, depending on the studied property, which is then used to relate the error of the estimation and the definition of the RVE size. As a result, confidence intervals of the effective properties, depending on the volume of calculations, are provided.

## **ARTIFICIAL “MAGNETIC ATOMS” FOR MICROWAVE COMPOSITE MATERIALS**

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Recently the fabrication and study of patterned magnetic structures became possible attracting large interest due to possible applications in new fields. One of these fields may concern microwave composite materials. From the point of view of fundamental studies, the reduction of dimensionality in microwave ferrites brings into play new effects, which should be described based on the quantized picture and demonstrate, as a fact, the properties of artificial atomic structures.

In a series of new publications, confinement phenomena of high-frequency magnetization dynamics in magnetic particles have been the subject of much experimental and theoretical attention (see e.g.[1]). Mainly, these works are devoted to the important studies of the magnetization spectra, but do not focus on the energy eigenstates of a whole ferrite-particle system. Till now there are no phenomenological models of a ferrite particle with high-frequency magnetization dynamics that use the effective-mass approximation and the Scrodinger-like equation to analyze *energy eigenstates* of a whole ferrite-particle system, similarly to semiconductor quantum wells.

The so-called magnetostatic (MS) oscillations in ferrite samples have the wavelength much less than the electromagnetic wavelength at the same frequency and, at the same time, much more than the exchange-interaction spin wavelength. This intermediate position between the “pure” electromagnetic and spin-wave (exchange-interaction) processes reveals very special behaviors of the geometrical effects. The confined effects for MS oscillations in normally magnetized thin-film ferrite disks demonstrate very unique properties. The  $\delta$ -functional (atomic-like) character of the multi-resonance MS spectra, one can observe experimentally in a ferrite disk resonator, leads to a clear conclusion that the energy of a source of a DC bias magnetic field is absorbing “by portions” or discretely, in other words. Contrary, the MS-wave spectrum of a ferrite sphere as well as the spin-wave spectra of magnetic particles shown in [1] are characterized by a very few and very “spreading” absorption peaks. Evidently, there should be a certain inner mechanism of quantization of the DC energy absorbed by a small disk-form ferrite sample. It was shown recently [2] that MS oscillations in a small ferrite disk resonator are described by the Schrödinger-like equation for MS-potential wave function and can be characterized by a discrete spectrum of energy levels. This fact allows analyzing the MS oscillations similarly to quantum mechanical problems. In this paper we give the results of energy spectrum calculations for MS oscillations in a ferrite disk resonator. Because of discrete energy eigenstates resulting from structural confinement in a special case of a normally magnetized ferrite disk, one can describe the oscillating system as a collective motion of quasi-particles – the “light magnons”. Effective masses of the “light magnons” are

calculated. Conformity of the “light-magnon” energy levels with the discrete levels of absorption energy is shown. A detailed analysis of the obtained results can be found in [3].

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## **Effective properties of matrix composite materials with high volume concentrations of inclusions (effective field approach)**

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The effective field method is applied to the calculation of the overall physical and mechanical properties of composite materials consisting of a homogeneous matrix and a set of isolated inclusions (two-phase media). The main hypothesis of the classical version of the method is the so-called quasicrystalline approximation. This hypothesis is the assumption that the field acting on every inclusion in the composite is constant and the same for all the inclusions. The predictions of this version of the method are in agreement with experimental data and numerical solutions for various effective properties of composites if the volume concentration of inclusions does not exceed 0.3. For higher volume concentrations of the inclusions, the method needs correction. In this work the version of the effective field method is developed for the improvement of the predictions of the effective properties of matrix composites in the region of high volume concentrations of inclusions. This version was outlined in previous works of the author, and is based on the detailed description of pair interactions between inclusions in the composite. In order to describe such interactions the hypothesis of the quasicrystalline approximation has to be changed for a more complex one. It gives an integral equation for the field that acts on a pair of inclusions in the composite medium. The kernel of the integral operator in this equation depends on a specific three-point correlation function of the random field of inclusions. The influence of this function on the overall dielectric properties of the composites is analyzed in 3D and 2D-cases. The predictions of the method are compared with numerical calculations of the effective dielectric properties of the two-phase composites in 2D-case.

# Hydrodynamics of "thermal" granular convection

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We employ the Navier-Stokes granular hydrodynamics for determining the threshold of "thermal" convection in a horizontal layer of fluidized granular medium [1]. In classical fluid the convection is driven by an externally imposed negative temperature gradient. In a fluidized granular medium a negative temperature gradient sets in spontaneously because of the energy loss by inelastic particle collisions. A recent experiment with a highly fluidized three-dimensional granular flow [2] gives strong evidence for thermal convection. In the simplest model of inelastic hard spheres, the convection sets in when the inelasticity coefficient  $q=(1-r)/2$  exceeds a critical value ( $r$  is the coefficient of normal restitution) [3]. In the hydrodynamic theory, the problem is fully described by three scaled parameters: inelasticity of particle collisions, the Froude number and the Knudsen number [4]. We find the dependence of the convection threshold, in terms of the inelasticity of particle collisions, on the Froude and Knudsen numbers. We also determine morphology of convection cells at the onset of convection. When the gravity is large enough, the Froude number drops out from the problem. When gravity goes to zero, the convection instability turns into a recently discovered phase separation instability [5-7]. A lower bound for the convection threshold is determined using the Schwarzschild criterion of stability of classical compressible fluid.

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# Diffusion mediated transport and the brownian motor

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Diffusion mediated transport is implicated in the operation of many molecular level systems. These include some liquid crystal and lipid bilayer systems, and, especially, the motor proteins responsible for eukaryotic intracellular traffic. All of these systems are extremely complex and involve subtle interactions on varying scales and are far from equilibrium. Here we explore the mechanisms underlying their far from equilibrium behavior and their relationship to transport including the formulation of a dissipation principle.

## ON THE EFFECTIVE CONSTANTS OF INHOMOGENEOUS POROELASTIC MEDIUM.

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The arbitrary anisotropic micro-inhomogeneous (composite) poroelastic medium is considered, containing a random set of ellipsoidal inclusions with other poroelastic characteristics. The properties of these constituents are described by the linear poroelastic theory by Biot [1,2]. One of the self-consistent schemes named effective field method (EFM) is used to develop the explicit expressions for the effective poroelastic characteristics (tensor of the frame elastic module  $C_{ijkl}^*$ , Biot's effective stress coefficient tensor  $\alpha_{ij}$  and Biot's constant  $M^*$ ) of the static poroelastic theory. For the two constituents composite porous materials these expressions satisfy the generalized Gassman relations obtained in [3,4]. Some special cases are considered for the isotropic main material (matrix).

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# **Force Chains and Stress in Granular Materials**

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The propagation of stress in granular materials remains a challenge to scientists, particularly in the limit of very hard grains. I will review a theory based on "force chains" -- linear paths of contacting grains which carry stress. The theory bridges the different scales of granular matter, from the small (grain) scale to the large (macroscopic) scale, via the mesoscopic scale which is common in experiments. I will discuss the full nonlinear theory as well as its linearized version, with an emphasis on response-function experiments.

# **NOISY REACTION-DIFFUSION MODELS AND THEIR BIOLOGICAL IMPLICATIONS**

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Reaction-diffusion processes arise in a wide variety of biophysical contexts ranging from intracellular signaling to pattern formation of microorganism colonies and to Darwinian evolutionary dynamics. In these processes, the discrete number of participating "individuals" (biological macromolecules, bacterial cells, or perhaps genomic types) can lead to stochastic fluctuations in what otherwise would be spatially-extended, nonlinear yet deterministic equations of motion. This talk will focus on several examples of phenomena in which this noise plays a primary role; these include cutoff effects in population genetics, noise-induced instabilities in models of bacterial colony growth, and nucleation-induced stochastic oscillations in cell calcium.

# **Switching Transitions in Liquid Crystal Composites**

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Switching transitions in confined liquid crystals differ from the Frederiks transition in homogeneous liquid crystal films. In polymer dispersed liquid crystals (PDLC), bipolar liquid crystal droplets, embedded in a polymer matrix, can be reoriented by an external field causing a change in the dielectric and optical properties of the composite. The transition threshold field is determined by the balance between the electrostatic energy of

the droplets and a strong anchoring elastic energy at the interface with the polymer. This balance may be studied analytically in some simple cases. As a result of the confined geometry, the threshold field does not depend on the thickness of the sample and splitting of the transition occurs in some situations. The sharpness of the transition may be controlled by varying the initial orientation distribution of the droplets. These effects may prove suitable for a wide range of electro-optic applications.

## **A transfer-matrix method for computing the macroscopic conductivity of three-constituent normal conductor/perfect insulator/perfect conductor random networks**

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We develop a transfer-matrix formulation to compute the conductivity of a normal conductor/perfect insulator/perfect conductor random network, and apply this approach in simulations of 2-dimensional and 3-dimensional networks. These simulations show that when a finite fraction of the normal conductor bonds in a random two-constituent percolating network are replaced by bonds of the third type, the critical behavior of the macroscopic conductivity remains unchanged. This wide universality of critical behavior in random networks is a crucial assumption in some recently published proofs of exact relations between elastic and electrical response of percolating networks [1,2].

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## **Pattern formation and thin water films**

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The appearance of patterns in non-equilibrium systems is the result of a nonlinear interaction between at least two different fields. There are many patterns which occur naturally in our everyday surroundings. In particular we will describe how patterns arise in thin water films evaporating from clean mica substrates. The films break up into coexisting

thick and thin regions, the boundaries between them showing dynamic patterns with features related to diffusion-limited growth in isotropic two-dimensional systems. We describe both experimental observations and a model for a volatile thin film bound to a substrate by competing Van der Waals and polar forces.

## **SOLUTION OF THE INHOMOGENEOUS HELMHOLTZ EQUATION FOR AN ELLIPSOIDAL SOURCE REGION**

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In the description of many dynamical problems in mathematical physics such as wave propagation in electrodynamics, acoustics or in the mechanics of materials (e.g. dynamic variant of Eshelby inclusion problem) the solution of the inhomogeneous Helmholtz equation (*dynamic- or 'Helmholtz potentials'*) for an ellipsoidal source region plays a key role. Surface integral representations are derived for inhomogeneous ellipsoids and ellipsoidal shells. As in the case of the static (Newtonian) potentials a compact representation of the *dynamic potentials* in terms of 1D integrals is highly desirable. Due to the mathematical complexity of the problem so far such representation seems to be absent in the literature. We close this gap for the dynamic potential for a homogeneous ellipsoidal shell for internal spacepoints. The derived solution of the inside region can easily be used to construct the solution outside of the ellipsoid by applying Ivory's theorem. For special cases such as spheres and circular continuous fibers, known closed form results are reobtained. In the static limit the approach provides a simple way to recover classical results of Ferrers (1877) and Dyson (1891) for the Newtonian potentials of ellipsoidal sources. The approach may be extended to construct 1D integral representations for the dynamic potentials of *inhomogeneous* ellipsoids and ellipsoidal shells.

# **Computational Mesomechanics of Materials: Virtual Testing of Microstructures and Possibilities of the Materials Optimization**

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The purpose of this work was to develop a concept of the computational material design at mesolevel and to demonstrate the realization of some steps of this concept as applied to Al/SiC composites. In the paper, a computational approach to the optimization of service properties of two-phase materials by varying their microstructure is presented. The main points of the optimization of composites include (1) the determination of the properties of the material constituents, and the deformation and fracture mechanisms, (2) numerical mesomechanical simulations of deformation, damage and fracture in idealized quasi-real microstructures of the composite, (3) the comparison of output parameters (stiffness, fracture resistances) of different microstructures and (4) the development of recommendations to the improvement of the microstructures of the materials [1-4].

Using a computational approach based on numerical experiments [5, 6], the author considered different microstructures of the particle reinforced metal matrix composite, and simulated the effect of the microstructures on their mechanical behavior and fracture resistance. The following arrangement of brittle inclusions in the materials were considered: uniform, net-like, clustered, gradient and layered arrangements, with different inclusion shapes (round, ellipsoids, etc.) and orientations. Crack paths for each of the microstructures were simulated, and the force-displacement curves were determined numerically.

The mechanisms of the toughening effect of the materials with the different microstructures are identified. It is demonstrated that extensive crack deviations from the initial cracking directions and the increase in the fracture toughness can be most efficiently achieved by using complex heterogeneous/localized microstructures, like clustered particle arrangements or alternated layers of fine and coarse inclusions.

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## **THE DYNAMICS OF SCREW DISLOCATIONS IN COPPER - A MOLECULAR DYNAMICS AND AN ELASTIC-CONTINUUM STUDY**

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The dynamics of dislocations constitutes one of the basic building blocks of any theory of plasticity. One of the methodologies to study plasticity is the bottom-up approach, in which rules for dislocations dynamics serve macroscopic continuum constitutive models. Experimental studies of dislocation motion are not able yet to follow in detail the microscopic dynamics of the dislocation. Using molecular dynamics methods the motion of dislocations under stress has been studied in detail for Cu as a function of both temperature and stress. A transition from inertial to viscous motion with a stress dependent terminal velocity has been observed. The experimentally observed stress dependence of the terminal velocity is reproduced quantitatively by our results. The dislocation structure is found to be time dependent with oscillations about the equilibrium structure. An elastic-continuum model, using a dislocation line model, was developed in order to study the simulation results by considering a simple model of dislocation motion consisting of an inertial line defect in an elastic medium with dissipation.

# **THE SOLID MECHANICS METHODS IN NANOTECHNOLOGICAL PROBLEMS**

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The problems of strength, problems of stability, problems of de-lamination etc. take place in traditional mechanics and in nanotechnology. Can we use the solid mechanics method in nano-technological problems? In present report it takes into account on some modification, which must be arrange for traditional methods a-priori. Then it is discussed the properties of composites with nano-dimensional grains, the quantum dots arrangement, the equilibrium of nano-tubeles and arrangement of nano-tubeles with help etching.

## **Mathematical modelling of two-dimensional phononic crystals**

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The problem considered is that of an infinite elastic medium containing a finite stack of gratings of circular cylindrical voids or elastic inclusions which are taken to be infinitely long and unidirectionally aligned parallel to the  $z$ -axis and spaced with period  $d$  along the  $x$ -axis. We assume that the void surfaces are free of tractions, and that the inclusions are either perfectly bonded to the surrounding medium, or connected to it via a thin and soft "coating" layer. We restrict ourselves here to the case of waves incident normally on the stack, so that the cross-polarisation effect is absent. We employ a multipole method to determine the reflection and transmission matrices for each grating, for both the scalar (out-of-plane shear) and vector (plane-strain) problems. These matrices are then used in a recurrence procedure to generate the scattering matrices for the entire stack which are then employed in numerical studies of band gaps or regions of inhibited propagation of elastic waves in the structure. We also present a generalisation of this method to study various forms of disorder within the array. The latter is introduced by treating gratings in which a macro-cell may contain several different inclusions, or inclusions and voids, and by varying the number of defects in each macro-cell, their position, radius and material constants from grating to grating, as well as the separation of gratings within the stack. Results are presented in the form of transmission diagrams exhibiting designs of structures with good low-pass and band-pass characteristics in transmission.

## **Convective Cahn-Hilliard models**

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Convective Cahn-Hilliard models have been suggested for the description of phase separation of driven systems and instabilities of crystallization fronts. With the increase of the driving force, a transition from the coarsening regime to a chaotic behavior takes place via a plethora of stable patterns characterized by a complex spatial structure but simple time dynamics. The relation of the dynamic transitions to the phenomenon of kinetic roughening of interfaces is discussed.

## **A phase field model with memory**

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A phase field model is proposed which incorporates the effects of slowly varying internal variables via a delayed or time averaged response of the system to the ambient driving forces. The internal variables we have in mind could model such effects as: (a) slow structural relaxation in a viscous solvent with a miscibility gap in the proximity of a glass transition temperature, or (b) clusters of impurity already segregated out from a mixture which might have a tendency to relax after quench.

We demonstrate that these memory effects can cause inertial effects giving rise for example to oscillation relaxation during grain shrinkage. The phase field model with memory can also be shown to be no more unstable than the classical phase field model, in an appropriate sense. Moreover, certain long time features of the system can be readily assessed via formal asymptotics.

## **Pattern formation, reconstruction, and roughening on a catalytic surface**

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Catalytic reactions on oriented single crystals often exhibit rate oscillations and produce a variety of spatio-temporal patterns on a micron scale. The most thoroughly studied

system of this kind is CO oxidation on Pt(110). The mechanism of rate oscillations and pattern formation under isothermal conditions at low pressure is based on a adsorbate-induced surface phase transition controlled by the CO coverage. The pattern formation on a micron scale can be modeled with the help of phenomenological mean-field equations containing a fraction of surface covered by one of the surface phases as a control variable. Mean-field theory cannot, however, capture many essential features of surface reconstruction, which involves material transport in a nanoscale range and is inadvertently linked to surface roughening.

We have carried out kinetic Monte-Carlo simulations of surface phase transitions on Pt(110) surface coupled to kinetic oscillations. Detailed data on bonding and activation energies of Pt atoms in different neighborhood configurations are extracted (and partly fitted and reconciled) from available ab initio computations and STM data, and used for computation of surface phase transitions and roughening. A realistic picture of kinetic oscillations and waves can be obtained with the help of a simplified Monte-Carlo model coupled to a mean field reaction-diffusion model.

## **Dynamical Instabilities of Quasi-static Crack Propagation Under Thermal Stress**

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We address the theory of quasi-static crack propagation in a strip of glass that is pulled from a hot oven towards a cold bath. This problem had been carefully studied in a number of experiments that offer a wealth of data to challenge the theory. We improve upon previous theoretical treatments in a number of ways. First, we offer a technical improvement of the discussion of the instability towards the creation of a straight crack. This improvement consists of employing Padé approximants to solve the relevant Wiener-Hopf factorization problem that is associated with this transition. Next we improve the discussion of the onset of oscillatory instability towards an undulating crack. We offer a novel way of considering the problem as a sum of solutions of a finite strip without a crack and an infinite medium with a crack. This allows us to present a closed form solution of the stress intensity factors in the vicinity of the oscillatory instability. Most importantly we develop a (*dynamical*) description of the actual trajectory in the regime of oscillatory crack. This theory is based on the dynamical law for crack propagation proposed by Hodgdon and Sethna. We show that this dynamical law results in a solution of the actual track trajectory in post critical conditions; we can compute from first principles the critical value of the control parameters, and the characteristics of the solution like the wavelength of the oscillations. We present detailed comparison with experimental measurements without any free parameter. The comparison appears quite excellent. Lastly we show that the dynamical law can be translated to an equation for the amplitude of the oscillatory crack; this equation predicts correctly the scaling exponents observed in experiments.

# **NON-HOMOGENIZATION APPROACH TO THE ANALYSIS OF PERIODIC CONTINUA: APPLICATIONS TO FRACTURE MECHANICS AND TOPOLOGICAL OPTIMIZATION**

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The knowledge of the effective moduli for a continuum with spatial periodicity in the geometric and elastic properties does not help one to determine the local stress strain field generated by a point force or a flaw. This stress field will be non-periodic in contrast to the field employed in the homogenization procedure. The problem is solved by the use of the representative cell method based on the discrete Fourier transform. The periodic elastic body is viewed as assemblage of arbitrary loaded identical modules perfectly bonded at their boundaries. The discrete Fourier transform with respect to the module number reduces the initial problem to the boundary value problem for a representative cell where the opposite boundaries are related by the Born-von Karman type boundary conditions. The obtained partial derivatives problem is formulated with respect to the complex valued transforms, but viewed as a usual elasticity problem. Consequently, it can be solved by any of the known analytical or numerical methods. The actual displacements in every point of the body are calculated than by the inverse transform integration. The above technique was applied for the solution of several fracture problems for bimaterial periodically layered composites. The violation of the periodicity by a single crack was overcome either by the use of the Wiener-Hopf method in the case of a semi-infinite crack or by derivation of the corresponding Green function for a single dislocation when the crack has finite length. Some interesting phenomena were observed. For example, it appeared that energy release rate for an interface crack is always less than the corresponding value for a crack between two dissimilar half planes only in the specific case when the thicknesses of all the layers are equal. Another application of the approach is in the field of topological optimization with multiple reanalysis. Consequently the efficiency of a single analysis becomes crucial. The problem for the representative cell in this case is solved numerically by the finite element method. Viewing the obtained optimal geometry of the infinite periodic structure as a microstructure of some material one can consider a new class of optimal materials characterized not by the extremum values of effective moduli but local optimal behavior.

# Plasmonic Nanoantennas

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Plasmonic nanomaterials open up the feasibility to detect molecules with We study the optical properties of metal nanocomposites and specially engineered metal nanostructures where an electromagnetic wave effectively couples to the surface plasmon modes. Such coupling leads to high local fields if the incident radiation resonantly excites the plasmon modes. Thus, metal nanostructured materials open new avenues for manipulating light and sensing molecules [1-5]. Engineered plasmonic structures can act as “smart” optical nano-antennas focusing light on nanometer scale areas, with high spatial and spectral control of the energy concentration. In this presentation, the optical properties of plasmonic nanomaterials and their novel applications in nano-photonics and spectroscopy will be discussed. We outline new phenomena in plasmonic nanomaterials, such as negative refraction [2,3,5], enhanced optical transmittance [1,4,5], plasmonic nano-lithography, disorder-induced localization of plasmons [1], and surface-enhanced nonlinear optical phenomena [1]. unsurpassed sensitivity and develop photonic nano-circuits allowing the control of photons in a similar manner as electrons are manipulated and controlled in conventional electronic circuits.

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# Variable Range Hopping (VRH) Conduction in Complex Systems and a Percolation Model (RRTN) with Tunneling

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The low-temperature ( $T$ ) electrical conductivity of a quantum insulator in  $d$ -dimensions given by the Mott's Variable Range Hopping (VRH) [1] formula, in its *general* form as:

$$\sigma(T) = \sigma_0 (T/T_0)^s \exp[-(T/T_0)^\gamma],$$

(the more popular form has  $s=0$ ), where  $T_0$  is a characteristic temperature-scale. For a disordered (non-interacting) solid,  $\gamma = 1/(d+1)$ . But, for an interacting (pure) system, Efros and Shklovskii [2] found that  $\gamma = 1/2$  independent of  $d$ . Some recent theoretical and experimental studies seem to indicate that there are systems for which the VRH-exponent  $\gamma$  is either (i) larger than any of the above predictions, (*e.g.*, in the experiment of ref. [3] on C-black-PVC composites  $\gamma = 0.67$ ; or, (ii) more intriguingly, as in the experiments of refs. [4,5],  $\gamma(p)$  is a continuous function of  $p$  (the dopant conc.), changing from about  $1/4$  to  $1$  (in 3D). Here we investigate the case (ii) with a semi-classical (or, semi-quantum) percolative behaviour where the *quantum tunneling* but, *no quantum-phase property*, is introduced; as in the RRTN (*Random Resistor cum Tunneling-bond Network*) model developed by us. With two phenomenological functions for the temperature ( $T$ )-dependence of the metallic and the semi-conducting bonds [6], we find quite satisfactorily that in the RRTN model (in 2D, for simplicity) as well, the VRH-exponent  $\gamma$  changes continuously with  $p$ . Of late, we have been studying the far-from equilibrium dynamics in the *driven* RRTN model. We may briefly discuss its two initial inverse-power-law (*cf.*, breakdown, avalanche, earthquake, bio-systems) dynamics, and a strong image recognition property in getting back to its natural (steady)state under a driving potential.

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# **Adaptation of autocatalytic reactants to discrete catalysts**

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Evolution of a system of diffusing and proliferating mortal reactants is analyzed in the presence of randomly moving catalysts. While the continuum description of the problem predicts reactant extinction as the average growth rate becomes negative, growth rate fluctuations induced by the discrete nature of the agents are shown to allow for an active phase, where reactants proliferate as their spatial configuration adapts to the fluctuations of the catalysts density. The model is explored by employing field theoretical techniques, numerical simulations and strong coupling analysis. For  $d \leq 2$ , the system is shown to exhibit an active phase at any growth rate, while for  $d > 2$  a kinetic phase transition is predicted. The applicability of this model as a prototype for a host of phenomena which exhibit self organization is discussed.

## **Effective characteristics of non-linear inhomogeneous media: Method of Local Linearization**

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A new approximate method, which allows analytical derivation of the effective conductivity of randomly inhomogeneous composites with non-linear IV characteristics phases, is described. Also this method is applied for description of materials with a hysteresis. In some cases, good agreement is shown with the previous results obtained by means of direct numerical and experimental methods.

# How Faithful are Continuum Models to Discrete Systems? Some Strange Rigorous Results and Their Obvious Real Life Applications

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Consider an infinite 2 dimensional world inhabited by 2 types of particles ("creatures"):

A ("angels"): they do not die, are not born and can only diffuse (jump randomly from one location to a neighboring one) with a probability rate  $DA$ . Assume they are initially distributed uniformly with a density  $R$ .

B ("mortals"): they diffuse too (with a probability rate  $DB$ ) and die with a probability rate  $M$ . In addition any pair A-B finding themselves on the same location can generate another B with probability rate  $L$  (cf. Genesis 6, 2-4).

The reaction-diffusion partial differential equations usually associated with such a system predict that the B's will eventually disappear exponentially whenever  $M > R L$ . However, it has been shown rigorously (both by renormalization group techniques and branching random walk theorems) that in fact the B population increases for any finite  $M$  and non-vanishing  $R$  and  $L$ .

This phenomenon is related to the discreteness of the agents and is the result of the spontaneous emergence of adaptive collective B objects that "search, follow and exploit" the local stochastic fluctuations in the A density. This mechanism has been related to a very wide range of emergent phenomena in complex systems in immunology, bacteria behavior, population biology, financial markets, economics, social sciences, propagation (and stopping) of social ills, marketing, computer networks, desertification and desert reclaim etc.

I will review the main idea and its applications in various fields.

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## **Exact Relations between Macroscopic Moduli of Composite Media in $n$ Dimensions**

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The macroscopic or bulk effective moduli of a composite medium depend on its detailed microstructure, and can usually be calculated only approximately. Notwithstanding this generic feature, there exist some exact, microstructure-independent results (known as Keller [1] or Dykhne theorem), which are valid only for strictly two-dimensional (2D) cases. Here we present generic  $n$ -dimensional ( $nD$ ) [in particular three-dimensional (3D)] exact relations between macroscopic or bulk effective moduli of composite systems with different microstructures [2]. These relations can be established between effective values of material coefficients of the same type (e.g. conductivity and conductivity) as well as

between different types of material coefficients (e.g. conductivity and permittivity). As an example of possible application of these relations, a set of Keller-like quasi-3D relations are derived for the case of columnar-shaped parallel inclusions. The microstructure in the two samples can, in general, be different. In particular, exact relations between bulk effective magneto-conductivity tensor components of a pair of composite samples with interchanged constituents and different columnar microstructures (as well as between two composites with the same host but different inclusions, e.g., perfectly insulating and perfectly conducting [2-3]) are found for general orientations of the applied magnetic field. Those relations are tested by comparing with a number of numerical calculations of macroscopic dc and ac response in such systems.

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## **Local fields and optical susceptibility of composite media**

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The developed earlier the generalized method of integral equations (GMIE) is applied to the problem of proper account of the local fields effects in inhomogeneous composite materials made in form of a microscopic or macroscopic mixture of several homogeneous components. The main idea GMIE stems from the supposition that a certain combination of the microscopic (local) fields, polarization vector, quadrupole, and magnetic-dipole volume densities and their gradients must satisfy both the integral and wave equations [1]. Under such an approach all tensor factors of these new quantities (variables) depend on the concrete structure of a given medium and are determined unambiguously. It allows us solve the problem of local factors and dielectric permittivity for arbitrary nonlinear and anisotropic homogeneous medium.

In the case of inhomogeneous media the effective dielectric permittivity turns out to be dependent not only on microscopic polarizabilities of the constituents but on degree of their mesoscopic aggregating (clustering). In the model of the spherical resonant impurities the result is compared with a case of the microscopically homogeneous doped medium. In the remarkable manner the clustering effects only in case of a vacuum host medium do not influence susceptibility of a composite whereas for any other host constituent the resonant impurities give rise to a strong enhancement of the effective permittivity. This result is a generalization of the well-known Maxwell Garnett model of a medium with allowance for the discrete nature of the sectional components. For the first time, the discrete characters of the impurities and host are taken into account on an equal footing. Heterogeneous composite materials such as optical fibers, semiconductor doped glasses, amorphous and polycrystalline semiconductors are widely used nowadays

everywhere. The obtained results suggest possibility of essential enhancement of the nonlinear susceptibility of microscopically heterogeneous composite materials.

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## **From Discrete to Continuum: Bridging Scales using Numerical Simulations**

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In this talk we discuss the passage from microscopic models to large scale continuum models using analysis combined with numerical simulations. We focus on fluids where the starting point is an atomistic model, using standard interaction potentials, such as Lennard-Jones potential. Discrete conservation laws are derived analytically, where certain fluxes are introduced. These fluxes and their dependence on temporal and spatial are studied using numerical simulation, resulting in closure relations. This results in intermediate scale stochastic models that are relevant for nonoscale fluid flow. These equations describe the evolution of the usual continuum mechanics averages, i.e., density, momentum and energy. As we pass to larger temporal and spatial scales, these stochastic terms diminish, and the models reduce to well known classical continuum equations, i.e., the Navier-Stokes equations. However, the evolution equations for kinetic and potential energy in this derivation are different from classical theory. An additional term representing transfer between these two forms of energy is derived, and may be important at certain scales. Issues and challenges regarding fluid mixtures will be addressed

## **INCLUSION BASED MODELLING OF CONCRETE WITH VARIOUS AGGREGATE VOLUME FRACTIONS**

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Fine and coarse particles play an important role in the mechanical properties of cementitious composites such as concrete. There is, however, little information available in the literature on the effects of type and volume fraction of particles on the mechanical properties of concrete. In this work, maximum particle size, the grading and the water-

cement ratio of concretes were kept constant, and the type and volume fraction of particles were varied from hardened cement paste to a workable concrete.

It has been shown that the toughening mechanisms are very important in the fracture energy of concrete. The fracture energies of all concretes were calculated based on meso-mechanical model. As the aggregate volume fraction increases, the modulus of elasticity, the splitting tensile strength, the effective stress intensity factor, the specific fracture energy and the characteristic length all increase, but the tensile strain capacity decreases and therefore, it can be concluded that this strain capacity is nearly independent of the type of aggregate within the limits of the presented work.

The compressive strength of concrete with coarse crushed limestone aggregates decreases as the aggregate volume fraction reaches up to a value of about  $0.30 \text{ m}^3/\text{m}^3$ , then increases significantly. In concretes with the rounded siliceous gravel, the compressive strength decreases substantially with the aggregate volume fraction. For the explanation of this behaviour, as seen in the enclosed figure, a model based on circular inclusions with the regular hexagonal symmetry in an infinite plate was proposed. The inclusions were all of equal radii and their centers were located at the center of the hexagonals. In a representative region of the plate, stress distributions were calculated using the collocation theory under far field uniform loads. It was seen that the calculated results by the theory are very close to the results obtained by the exact solution in the case of single inclusion. In addition, theoretically known isotropy of the plate in the large scale was also determined by the proposed model. Based on this model, it can be concluded that the stress concentrations increase at the weak matrix-aggregate interfaces as the volume fraction of aggregate in the mixture increases. This increase in the stress concentration may be responsible from the drop of the compressive strength. For the aggregate volume fractions greater than  $0.30 \text{ m}^3/\text{m}^3$ , the number of crushed limestone aggregates in the vertical cross-sectional planes reach a sufficient level. The vertical cracks grow through the aggregates and since the tensile strength of limestone aggregate is greater than that of the matrix, the compressive strength increases with the increase in the aggregate volume fraction. There is still the augmentation of stress concentration with the aggregate volume fraction at the aggregate-matrix interfaces, however, the beneficial effect raising from cracks growing through the aggregates is dominant. In case of concretes with rounded siliceous gravel, these aggregates with smooth surface may play a negative role in compression where several fracture planes may develop parallel to the loading axes in the three-dimensional case, whereas in splitting and bending tests, the crack may be forced to pass through the aggregate in a specific fracture plane.

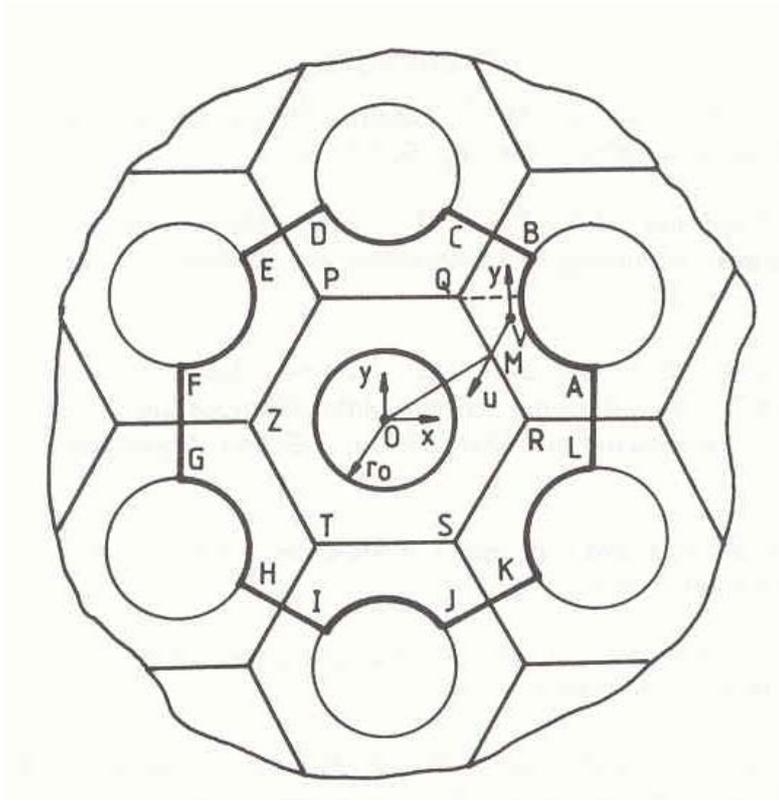


Figure. Circular inclusions with respect to the regular hexagonal symmetry

## **On the Approximation Theorem for Functionals and the Asymptotic Stability for Some Classes of Polynomial Fluids**

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In this paper we prove that if the polynomial fluids are not considered as some approximations obtained by means of the "Approximation Theorem for Functionals", of Coleman and Noll (see Joseph 1974, 1981), then (at least for third grade fluids) the rest state is asymptotically stable (for any  $\alpha_1$ ). For this, we briefly remind first some known results concerning the asymptotic stability of the rest state for second and third grade fluids (Fosdick and Rajagopal (1973), Fosdick and Straughan (1981), Joseph for instance) in order to understand the influence, onto these results, of the famous Coleman and Noll's Approximation Theorem for Functionals ((1960) which is one of the mathematical ways to introduce polynomial constitutive laws for fluids). It is known after Joseph's papers that polynomial fluids "of grade  $n > 1$  does not exist" (in the sense the specific coefficients  $\alpha_1, \beta_1, \dots$  of higher orders Rivlin-Ericksen tensors must vanish) if we apply the mentioned theorem and if we demand also, that the second law of thermodynamics (in the sense of Clausius and Duhem) be satisfied. In this context it was proved (in various ways) that the

rest state does not be asymptotically stable (some “anomalous futures” are present in second grade fluids for  $\alpha_1 < 0$ , for instance. See cited papers and Huilgol and Phan Thien (1986) also). After that we pass to present some results of Tigoiu (2000, 2001, 2002). These one are referring to third grade fluids. Here it was considered only those restrictions imposed on a third grade fluid by the second law of thermo-dynamics and then, under some restrictions on the constitutive modules (in correlation to the dimensions of the flow domain), it results that the rest state is asymptotically stable (for weakly perturbed flows). In the last part of our work we prove that the rest state is asymptotically stable for general motions and for any  $\alpha_1$ .

Finally we remark also that this kind of problems (approximates, in some asymptotic expansions, which does not have all the properties of the approximated function) is not singular in the range of Mechanics and Thermodynamics. Indeed, at least one other very important example is well known and is produced by the so called Chapman and Enskog expansion from the Kinetic Theory of Gases (which provides in the first two steps of approximation macroscopic constitutive laws which are objective and at the third step of approximation, a macroscopic law which is not objective). Consequently, we conclude that, in order to a third grade fluid be asymptotically stable in his rest state (and than be correctly described by the known polynomial law) for any  $\alpha_1$ , it is necessary that  $\beta_1 < 0$ .

## **The lattice-gas model in micro-aero-hydrodynamic problems: Applications to molecular flows in narrow pores and contact line motions on open surfaces**

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At present, the dynamics of transport for the mass, momentum and energy in nanoscaled systems (nanopores and contact line motions) for time intervals more than  $10^{-7}$  -  $10^{-6}$  s is usually treated in terms of Navier-Stocks equation. However, this description is questionable because of the strong fluid inhomogeneity in nanopores as well as contact line movements on open surfaces because of the surface potential, and in case of a menisci formation at the vapor-liquid interface in pores due to molecular interactions.

At last time new numerical technique for molecular level investigations on nanoscale temporal and spatial domains have been developed [1-3], which allows to consider various molecular flows in porous systems and for open surfaces during time intervals from  $10^{-11}$  -  $10^{-9}$  seconds up to  $10^{-5}$  -  $10^{-4}$  seconds. We were used the kinetic theory for the lattice-gas model. The lattice-gas model is the simplest molecular model of the dynamics on the microscopic level. This model takes into account all molecular forces and covers a wide range of fluid densities (from the gaseous up to the liquid state) and temperatures, including the critical range [4,5].

The main advantage of atomic-molecular kinetic equations is that they can be used practically for all times, beginning from microscopic scale (from a characteristic time of atom oscillations) up to macroscopic times, including equilibrium condition of a system [5,6] (kinetic equation for processes in a condensed phase has the Glauber's type equations [7].)

In the lattice-gas model, it is easy to account for correlation effects; therefore this model has a strong advantage over the Boltzmann equation, where only the unary distribution function is used and correlation effects between lateral interacting molecules are absent. The non-equilibrium pair distribution function plays the main role in these new equations, since the form of the equations for the pair distribution function changes at various spatial scales.

The lattice-gas model has some advantages for solving the problem formulated above. First, it provides a self-consistent description of both equilibrium and dynamic properties of the system in a wide range of time scales (starting from the pico-second interval). Second, the calculation based on this model can be performed more rapidly, compared to other numerical methods. Third, the model is in full quantitative agreement with the MD and Monte Carlo simulations in the whole parameter range of the phase diagram, excluding critical points where a qualitative agreement can be achieved, as well as agreement with MD simulation and kinetic theory of inhomogeneous fluids [8].

On basis of the kinetic theory (the Master Equation) the Navier - Stokes type equations were constructed for local equations for the concentration, momentum and energy transfer. Corresponding expressions for concentration dependences of following dissipative factors: selfdiffusion, shear and volume viscosity, as well as thermal conductivity have been obtained. The numerical analysis of the Navier - Stokes type equations are executed by a "relaxation" method of the second order of accuracy on temporary and space coordinates.

Using the new approach, we have analyzed the dynamic modes of flows for argon atoms in slit shaped pores in a wide range of densities, including those at which the adsorbed fluid undergoes vapor-liquid separation. At low fluid densities we have obtained a strong anisotropic distribution of fluid on normal to surfaces of pore walls due to adsorption forces. Profiles of speed distributions for flows in pores have been found to differ from the Poiseuille's flow. When the state of the fluid in a nanopore is vapor-like, no viscous flow is observed. When the state of the fluid is liquid-like, the anisotropy of the fluid across the pore was less pronounced, and a volume flow was observed.

Using this technique, the dynamic of wetting of a graphite slab by liquid argon was modeled. A detailed study has been performed of the dynamics of the three phase contact line before the steady state regime was established. The velocity of the contact line motion along the Wilhelmy plate is found to decrease as the depth of the solid-fluid potential decreases. In the vicinity of the three-phase contact, the vapor-liquid interface was non-stationary, and formed a foam-type structure. The front of the foam extended along the vapor-liquid and liquid-solid interface. At a lower temperature, the foaming effect was less pronounced.

Perspectives of the given approach for describing the dynamics of liquid flows which contain large particles (such as surfactants, fluid suspensions, albumens, etc. ) will be discussed.

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## **Computation of ground bearing capacity from shear wave velocity**

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Ground bearing capacity, which stands for the maximum pressure that the base can bear without collapsing, depends on mechanical features such as ground's weight per unit volume, shear strength and deformation characteristics; on the initial tension status and hydrolic conditions and on the geometrical and physical conditions such as depth, shape and load the base bears. Traditional method is to use the ground bearing capacity formula of Terzaghi.

Ground bearing capacity can be computed by substituting the data from the results of soil mechanics laboratory and field experiments to Terzaghi's formula. Among field experiments, SPT (Standard Penetration Test) is included.

If the strong relationships between shear wave velocity of Imai and Yoshimura (1975) and the SPT; and between shear wave velocity and unconfined pressure strength are taken into account, ground bearing capacity can be computed from shear wave velocity.

Ground bearing capacity can be calculated from the relation:

$$q(f)=V(s)*\gamma*T(0)/4 \text{ kg/cm}^2$$

and safe bearing capacity can be computed from:

$$q(a)=q(f)/3$$

This method is compatible with classical Terzaghi method.

# **BOUNDARY ELEMENT METHOD APPLICATION TO SOME MULTIPHASE FLOWS**

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Multiphase flows are one of the most difficult and complex problems of modern hydrodynamics. Complexity of such flows is a result of hydrodynamic interaction between small objects of second phase (and possible third) with main phase and among them. There are two well-known kinds of flows from the point of view of hydrodynamic interaction: the first one is a flow with one or several large objects, which determine the flow scale, and the second one is a flow with a lot of small objects of second phase. The first kind of problems is successfully solvable by traditional numerical methods. The second kind of problems is well investigated in asymptotic approximation, assuming that the second phase objects are asymptotically small and they create a continuous phase. A lot of problems with non-asymptotically small second phase remain outside two mentioned cases, as a result, they are investigated not so good as mentioned problems.

The traditional numerical methods cannot be used for a numerical solution of problems in principle, because they cannot provide any information about a process, whose reference size is less than the cell size. The most natural approach to considering problem is Lagrangian consideration of second phase object motion. One of the most successful works in this direction was attempt to apply discrete vortices method to the main flow calculation with calculation of individual motion of any second phase particles. In the present work combined boundary element and discrete vortices method is applied. Specific boundary element method algorithm with integration along real boundary is used, what improved the calculation accuracy of object motion near solid boundaries.

Consider the problem of interaction between the objects. Complete calculation of every interaction is impossible due to very large number of such interactions. However single interaction can be calculated in detail. The simplest way to avoid of individual calculation of every interaction is replacement of such calculation by “scenario” of interaction. If there are finite kind of objects, there are finite number of “scenarios” of their interactions. Some such “scenarios” can be constructed even without complete calculation of interaction. Not only deterministic, but also stochastic “scenarios” can be introduced. Using of “scenarios” sufficiently saves a required computer time and other computer resources.

As an example of application of proposed approach consider a multiphase flow with non-asymptotically small objects of second phase. Solid particles in any flow, liquid drops in gas flows and gas bubbles in fluid flows can be considered as second phase objects. On the macro level motion of second phase objects is modeled by motion of material points and their influences on the flow are modeled by discrete singularities on far distances. For small distances the main field isn't considered of any specific way, because it is assumed that the discrete singularity doesn't influence on the field in the point, where it is situated. Consideration of interaction on small distance is replaced by “scenario”. Besides of that there are possible different vortical structures in the flow, which are represented by discrete vortices. Interaction between second phase objects and discrete vortices is considered by the same way. Generally speaking material singularities (solid particles, liquid drops or gas bubbles) and kinematic singularities (discrete vortices, sources, dipoles) influence on main

flow. Proposed approach gives an opportunity to take into account effects of any geometrical (and temporary for non-stationary processes) scales in single computational scheme.

The proposed approach is illustrated by several examples of numerical calculation of plane multiphase flows, in particular by the problem about spraying of protective coating.

## **Diversity of Vegetation Patterns and Desertification**

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A large-scale view of arid regions often shows that the vegetation grows in patterns. These are related to the amount of precipitation as well as to the topography. A model will be presented that reproduces the wide range of patterns observed in water-limited regions, from bare soil at very low precipitation to uniform cover at high precipitation, through intermediate states of spot-, stripe- and hole-patterns. The model predicts the coexistence of more than one stable state in a given range of precipitation. The results of the model lead to an understanding of the hysteretic nature of desertification, and to a new approach to the classification of aridity.

## **The effective properties of macroscopically inhomogeneous ferromagnetic composites**

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Various theoretical models (self-consistent field, local linearization, and percolation theory methods and an analytic solution of the linear problem for an ordered medium) for calculating the magnetostatic properties of two-phase composites containing one ferromagnetic phase were considered. The concentration and field dependences of the effective magnetic permeability were found. A method for determining the coercive force and remanent magnetization as functions of the ferromagnetic phase concentration was suggested. The results were compared with experimental data.