Computing thermal effects on nonlinear optical properties of small atoms

The significance of nonlinear optical properties (NOP) is pronounced in many physical scales starting from microscopic interactions, such as van der Waals, to macroscopic properties, like dielectric constant and refractive index. Obtaining NOP, that is, dipole and multipole moments and (hyper)polarizabilities of matter, by computational simulation is particularly important in systems beyond experimental reach, such as exotic light-nucleus molecules in warm dense matter present in stars and gas planets, or short life-time particles such as positron. Most first-principles approaches are straightforward in 0 K but become tedious in thermal ensembles and beyond the adiabatic approximation.

The path-integral Monte Carlo method (PIMC) provides a tangible interface between the tensorial and the thermally averaged character of molecular (hyper)polarizabilities. In a recent study [1], we have derived field-free estimators that make the computation even more straightforward than our previous finite-field approach [2]. With the adiabatic, i.e. Born–Oppenheimer, approximation we obtain accurate tensorial ground state (hyper)polarizabilities, while the nonadiabatic simulation adds in considerable rovibrational effects and thermal coupling. In case of several two-electron systems, our results at the 0 K limit are either novel or in excellent agreement with the literature (e.g., see Fig. 1). Besides these results, we are presenting the derivation and demonstration of yet unpublished estimators for dipole-quadrupole polarizabilities of small molecules.

Active Learning for Sound Event Classification by Clustering Unlabeled Data

This paper proposes a novel active learning method to save annotation effort when preparing material to train sound event classifiers. K-medoids clustering is performed on unlabeled sound segments, and medoids of clusters are presented to annotators for labeling. The annotated label for a medoid is used to derive predicted labels for other cluster members. The obtained labels are used to build a classifier using supervised training. The accuracy of the resulted classifier is used to evaluate the performance of the proposed method. The evaluation made on a public environmental sound dataset shows that the proposed method outperforms reference methods (random sampling, certainty-based active learning and semi-supervised learning) with all simulated labeling budgets, the number of available labeling responses. Through all the experiments, the proposed method saves 50–60% labeling budget to achieve the same accuracy, with respect to the best reference method.

Quantum Monte Carlo methods from ground state to thermal equilibrium and real-time propagation of electronic structure
A conceptual modeling and simulation framework for system Design

This article presents the dimensional analysis conceptual modeling (DACM) framework, intended as a conceptual modeling mechanism for lifecycle systems engineering. DACM is a novel computer-aided method originally developed for military projects, but it's now available for other applications, too. The DACM framework is a powerful approach for specifying, discovering, validating, and reusing building blocks as well as analyzing system behavior in early development stages. This framework is based on dimensional analysis combined with causal graphs to represent the interactions and interdependencies among system variables. The framework's algorithms are codified into software applications to facilitate its use. This article provides a practical presentation of the steps that encompass the transformation from problem to solution space, key system variables extraction, causal ordering, clustering of variables, and qualitative analyses. The authors provide two examples that cover in detail the DACM's mathematic machinery for deriving a system's behavioral laws from a causal graph. The entire DACM approach is supported by a computer-based application that integrates all the steps of the framework presented in this article.
Photoexcitation and electron transfer at inorganic–organic interface — a DFT approach

General information
State: Published
Organisations: Department of Physics, Research group: Electronic Structure Theory, Research area: Computational Physics, Department of Chemistry and Bioengineering
Authors: Niskanen, M. O., Kontkanen, O. V., Hukka, T. I., Rantala, T. T.
Number of pages: 1
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Peer-reviewed: Unknown
Event: Paper presented at Optics and Photonics days, Tampere, Finland.
Research output: Scientific › Paper, poster or abstract

Finite temperature path-integral modeling of quantum dot cellular automata

General information
State: Published
Organisations: Department of Physics, Research group: Semiconductor Technology and Applications, Optoelectronics Research Centre, Research area: Computational Physics, Research group: Electronic Structure Theory
Authors: Tiihonen, J., Schramm, A., Kylänpää, I., Rantala, T.
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Path integral simulation of eigenstates and dynamics of electrons

General information
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Organisations: Department of Physics, Research group: Electronic Structure Theory, Research area: Computational Physics
Authors: Ruokosenmäki, I. S., Gholizadeh kalkhoran, H., Kylänpää, I. T., Rantala, T. T.
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Bill2d: A software package for classical two-dimensional Hamiltonian systems
We present Bill2d, a modern and efficient C++ package for classical simulations of two-dimensional Hamiltonian systems. Bill2d can be used for various billiard and diffusion problems with one or more charged particles with interactions, different external potentials, an external magnetic field, periodic and open boundaries, etc. The software package can also calculate many key quantities in complex systems such as Poincaré sections, survival probabilities, and diffusion coefficients. While aiming at a large class of applicable systems, the code also strives for ease-of-use, efficiency, and modularity for the implementation of additional features. The package comes along with a user guide, a developer's manual, and a documentation of the application program interface (API). Program summary Program title: Bill2d Catalogue identifier: AEYL_v1.0 Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEYL_v1.0.html Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland Licensing provisions: GNU General Public License, version 3 No. of lines in distributed program, including test data, etc.: 37098 No. of bytes in distributed program, including test data, etc.: 1155037 Distribution format: tar.gz Programming language: C++(14). Computer: Tested on x86 and x86 64 architectures. Operating system: Tested on Linux, and OS X versions 10.9 and 10.10. Has the code been vectorised or parallelized?: Shared memory parallelization when simulating ensembles of systems. RAM: Simulation
dependent: kilobytes to gigabytes Classification: 4.3, 7.8, 7.9, 7.10, 16.9. External routines: Boost, CMake, GSL, HDF5; and optionally Google-Mock, GoogleTest, and Doxygen Nature of problem: Numerical propagation of classical two-dimensional single and many-body systems, possibly in a magnetic field, and calculation of relevant quantities such as Poincaré sections, survival probabilities, diffusion co-efficients, etc. Solution method: Symplectic numerical integration of Hamilton’s equations of motion in Cartesian coordinates, or solution of Newton’s equations of motion if in a magnetic field. The program implements several well-established algorithms. Restrictions: Pointlike particles with equal masses and charges, although the latter restrictions are easy to lift. Unusual features: Program is efficient, extremely modular and easy to extend, and allows arbitrary particle–particle interactions. Additional comments: The source code is also available at https://bitbucket.org/solanpaa/bill2d. See README for locations of user guide, developer manual, and API docs. Running time: From milliseconds to days, depends on type of simulation.

General information
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Organisations: Department of Physics, Research group: Quantum Control and Dynamics
Authors: Solanpää, J., Luukko, P., Räsänen, E.
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Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 2.136 2.224
Publication Forum (2016): 1
Scopus rating (2015): 1.816 2.185
Web of Science (2015): 3.635 3.553 7.5 0.888 0.03222 1.432
Publication Forum (2015): 1
Scopus rating (2014): 1.35 1.682
Web of Science (2014): 3.112 3.508 8.0 1.19 0.03227 1.426
Publication Forum (2014): 1
Scopus rating (2013): 1.47 1.729
Publication Forum (2013): 1
Scopus rating (2012): 2.122 2.136
Publication Forum (2012): 1
Scopus rating (2011): 1.749 1.929
Scopus rating (2010): 1.469 1.394
Scopus rating (2008): 1.232 1.156
Scopus rating (2007): 0.99 1.075
Scopus rating (2006): 1.018 1.132
Scopus rating (2005): 0.753 1.135
Scopus rating (2004): 0.961 1.095
Scopus rating (2003): 0.941 0.962
Scopus rating (2002): 0.657 0.84
Scopus rating (2001): 0.591 0.848
Scopus rating (2000): 0.845 0.84
Scopus rating (1999): 1.226 1.027
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DOIs: 10.1016/j.cpc.2015.10.006
Source: RIS
Source-ID: urn:47AC3DE9B47E65408DED4F825269FF66
Research output: Scientific - peer-review » Article
Cis and Trans Unsaturated Phosphatidylcholine Bilayers: A Molecular Dynamics Simulation Study

Trans unsaturated lipids are uncommon in nature. In the human diet, they occur as natural products of ruminal bacteria or from industrial food processing like hydrogenation of vegetable oils. Consumption of trans unsaturated lipids has been shown to have a negative influence on human health; in particular, the risk of cardiovascular disease is higher when the amount of trans unsaturated lipids in the diet is elevated. In this study, we first performed quantum mechanical calculations to specifically and accurately parameterize cis and trans mono-unsaturated lipids and subsequently validated the newly derived parameter set. Then, we carried out molecular dynamics (MD) simulations of lipid bilayers composed of cis or trans unsaturated lipids with and without cholesterol. Our results show that trans mono-unsaturated chains are more flexible than cis mono-unsaturated chains due to lower barriers for rotation around the single bonds next to the trans double bond than those next to the cis double bond. In effect, interactions between cholesterol and trans unsaturated chains are stronger than cis unsaturated chains, which results in a higher ordering effect of cholesterol in trans unsaturated bilayers.

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Authors: Kulig, W., Pasenkiewicz-Gierula, M., Róg, T.
Keywords: (cholesterol, OPLS-AA force field, torsional potential, model validation)
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Journal: Chemistry and Physics of Lipids
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Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.976 0.862
Publication Forum (2016): 1
Scopus rating (2015): 0.957 0.957
Web of Science (2015): 2.901 2.75 >10.0 0.868 0.00491 0.736
Publication Forum (2015): 1
Scopus rating (2014): 0.885 1.039
Web of Science (2014): 2.422 2.697 >10.0 1.233 0.00529 0.788
Publication Forum (2014): 1
Scopus rating (2013): 0.82 1.055
Publication Forum (2013): 1
Scopus rating (2012): 0.803 0.974
Publication Forum (2012): 1
Scopus rating (2011): 0.727 0.984
Scopus rating (2010): 0.874 0.964
Scopus rating (2009): 0.9 0.995
Scopus rating (2008): 1.114 1.057
Scopus rating (2007): 1.083 1.091
Scopus rating (2006): 0.808 0.881
Scopus rating (2005): 1.038 1.035
Scopus rating (2004): 0.69 0.831
Scopus rating (2003): 0.917 0.817
Scopus rating (2002): 1.005 0.813
Scopus rating (2001): 1.097 0.827
Scopus rating (2000): 0.738 0.742
Scopus rating (1999): 0.737 0.705
Original language: English
DOIs:
10.1016/j.chemphyslip.2015.07.002
Long-range correlations and burstiness in written texts: Universal and language-specific aspects

Recently, methods from the statistical physics of complex systems have been applied successfully to identify universal features in the long-range correlations (LRCs) of written texts. However, in real texts, these universal features are being intermingled with language-specific influences. This paper aims at the characterization and further understanding of the interplay between universal and language-specific effects on the LRCs in texts. To this end, we apply the language-sensitive mapping of written texts to word-length series (wls) and analyse large parallel (of same content) corpora from 10 languages classified to four families (Romanic, Germanic, Greek and Uralic). The autocorrelation functions of the wls reveal tiny but persistent LRCs decaying at large scales following a power-law with a language-independent exponent $\sim 0.60-0.65$. The impact of language is displayed in the amplitude of correlations where a relative standard deviation $>40\%$ among the analyzed languages is observed. The classification to language families seems to play a significant role since, the Finnish and Germanic languages exhibit more correlations than the Greek and Roman families. To reveal the origins of the LRCs, we focus on the long words and perform burst and correlation analysis in their positions along the corpora. We find that the universal features are linked more to the correlations of the inter-long word distances while the language-specific aspects are related more to their distributions.

General information
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Organisations: Department of Physics, Research area: Computational Physics
Authors: Constantoudis, V., Kalimeri, M., Diakonos, F., Karamanos, K., Papadimitriou, C., Chatzigeorgiou, M., Papageorgiou, H.
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Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.324 0.364
Publication Forum (2016): 1
Scopus rating (2015): 0.36 0.371
Web of Science (2015): 0.85 0.582 8.3 0.199 0.00559 0.2
Publication Forum (2015): 1
Scopus rating (2014): 0.379 0.421
Web of Science (2014): 0.937 0.519 7.8 0.293 0.0062 0.181
Publication Forum (2014): 1
Scopus rating (2013): 0.265 0.341
Publication Forum (2013): 1
Scopus rating (2012): 0.231 0.273
Publication Forum (2012): 1
Scopus rating (2011): 0.231 0.342
Scopus rating (2010): 0.243 0.323
Scopus rating (2009): 0.326 0.393
Scopus rating (2008): 0.357 0.354
Scopus rating (2007): 0.426 0.435
Scopus rating (2006): 0.301 0.386
Scopus rating (2005): 0.51 0.359
Scopus rating (2004): 0.363 0.319
Scopus rating (2003): 0.363 0.338
Scopus rating (2002): 0.46 0.389
Scopus rating (2001): 0.494 0.386
Magnetic cotton yarns: optimization of magnetic properties

In this paper, we present the effect of ferrite percentage content and electric current intensity passing through the electromagnet coil on magnetic properties (saturation induction, residual induction, and coercive field) of magnetic staple yarns. Also, we present a method for obtaining magnetic yarns by direct coating with magnetic powder (barium ferrite). The aim of the study is to determine the optimal processing factors that can affect the performance of magnetic characteristics using an experimental design for second-order model. The results show that an increase in ferrite percentage content is influencing the saturation and residual induction more than an increase in applied current intensity. The increase in saturation and residual induction is due to the higher content of ferrite powder from the magnetic solution that adheres on the yarn surface. The higher is the value of coercive field, the larger is the force needed to completely demagnetize the magnetic yarn.
Role of charged lipids in membrane structures: Insight given by simulations

Lipids and proteins are the main components of cell membranes. It is becoming increasingly clear that lipids, in addition to providing an environment for proteins to work in, are in many cases also able to modulate the structure and function of those proteins. Particularly charged lipids such as phosphatidylinositol and phosphatidylserines are involved in several examples of such effects. Molecular dynamics simulations have proved an invaluable tool in exploring these aspects. This so-called computational microscope can provide both complementing explanations for the experimental results and guide experiments to fruitful directions. In this paper, we review studies that have utilized molecular dynamics simulations to unravel the roles of charged lipids in membrane structures. We focus on lipids as active constituents of the membranes, affecting both general membrane properties as well as non-lipid membrane components, mainly proteins. This article is part of a Special Issue entitled: Biosimulations edited by Ilpo Vattulainen and Tomasz Róg.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, University of Helsinki, University of Southern Denmark
Authors: Pöyry, S., Vattulainen, I.
Keywords: (Cardiolipin, Lipid membrane, Lipid-protein interactions, Phosphatidylinositol, Phosphatidylserine)
Number of pages: 12
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ASJC Scopus subject areas: Biochemistry, Cell Biology, Biophysics

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Publication Forum (2017): 1
Scopus rating (2016): 1.511 1.101
Publication Forum (2016): 1
Scopus rating (2015): 1.782 1.142
Web of Science (2015): 3.687 3.589 7.3 0.907 0.02731 1.163
Publication Forum (2015): 1
Scopus rating (2014): 1.869 1.09
Web of Science (2014): 3.836 3.881 7.0 1.006 0.02991 1.257
Publication Forum (2014): 2
Scopus rating (2013): 1.592 0.975
Publication Forum (2013): 2
Scopus rating (2012): 1.833 1.156
Publication Forum (2012): 2
Scopus rating (2011): 1.644 1.227
Scopus rating (2009): 2.152 1.298
Scopus rating (2008): 2.035 1.123
What can we learn about cholesterol's transmembrane distribution based on cholesterol-induced changes in membrane potential?

Cholesterol is abundant in the plasma membranes of animal cells and is known to regulate a variety of membrane properties. Despite decades of research, the transmembrane distribution of cholesterol is still a matter of debate. Here we consider this outstanding issue through atomistic simulations of asymmetric lipid membranes, whose composition is largely consistent with eukaryotic plasma membranes. We show that the membrane dipole potential changes in a cholesterol-dependent manner. Remarkably, moving cholesterol from the extracellular to the cytosolic leaflet increases the dipole potential on the cytosolic side, and vice versa. Biologically this implies that by altering the dipole potential, cholesterol can provide a driving force for cholesterol molecules to favor the cytosolic leaflet, in order to compensate for the intramembrane field that arises from the resting potential.
Topologies, structures and parameter files for lipid simulations in GROMACS with the OPLS-aa force field: DPPC, POPC, DOPC, PEPC, and cholesterol

In this data article we provide topologies and force field parameters files for molecular dynamics simulations of lipids in the OPLS-aa force field using the GROMACS package. This is the first systematic parameterization of lipid molecules in this force field. Topologies are provided for four phosphatidylcholines: saturated DPPC, mono-cis unsaturated POPC and DOPC, and mono-trans unsaturated PEPC. Parameterization of the phosphatidylcholines was achieved in two steps: first, we supplemented the OPLS force field parameters for DPPC with new parameters for torsion angles and van der Waals parameters for the carbon and hydrogen atoms in the acyl chains, as well as new partial atomic charges and parameters for torsion angles in the phosphatidylcholine and glycerol moieties [1]. Next, we derived parameters for the cis and trans double bonds and the neighboring them single bonds [2]. Additionally, we provide GROMACS input files with parameters describing simulation conditions (md.mdp), which are strongly recommended to be used with these lipids models. The data are associated with the research article “Cis and trans unsaturated phosphatidylcholine bilayers: a molecular dynamics simulation study” [2] and provided as supporting materials.

Segregation, precipitation, and α−α′ phase separation in Fe-Cr alloys

Iron-chromium alloys, the base components of various stainless steel grades, have numerous technologically and scientifically interesting properties. However, these features are not yet sufficiently understood to allow their full exploitation in technological applications. In this work, we investigate segregation, precipitation, and phase separation in Fe-Cr systems analyzing the physical mechanisms behind the observed phenomena. To get a comprehensive picture of Fe-Cr alloys as a function of composition, temperature, and time the present investigation combines Monte Carlo simulations using semiempirical interatomic potential, first-principles total energy calculations, and experimental spectroscopy. In order to obtain a general picture of the relation of the atomic interactions and properties of Fe-Cr alloys in bulk, surface, and interface regions several complementary methods have to be used. Using the exact muffin-tin orbitals method with the coherent potential approximation (CPA-EMTO) the effective chemical potential as a function of Cr content (0−15 at. % Cr) is calculated for a surface, second atomic layer, and bulk. At ~10 at. % Cr in the alloy the reversal of the driving force of a Cr atom to occupy either bulk or surface sites is obtained. The Cr-containing surfaces are expected when the Cr content exceeds ~10 at. %. The second atomic layer forms about a 0.3 eV barrier for the migration of Cr atoms between the bulk and surface atomic layer. To get information on Fe-Cr in larger scales we use semiempirical methods. However, for Cr concentration regions less than 10 at. %, the ab initio (CPA-EMTO) result of the important role of the second atomic layer to the surface is not reproducible from the large-scale Monte Carlo molecular dynamics (MCMD) simulation. On the other hand, for the nominal concentration of Cr larger than 10 at. % the MCMD simulations show the precipitation of Cr into isolated pockets in bulk Fe-Cr and the existence of the upper limit of the solubility of Cr into Fe layers in Fe/Cr layer systems. For high Cr concentration alloys the performed spectroscopic measurements support the MCMD simulations. Hard x-ray photoelectron spectroscopy and Auger electron spectroscopy investigations were carried...
out to explore Cr segregation and precipitation in the Fe/Cr double layer and Fe0.95Cr0.05 and Fe0.85Cr0.15 alloys. Initial oxidation of Fe-Cr was investigated experimentally at 10−8 Torr pressure of the spectrometers showing intense Cr2O3 signal. Cr segregation and the formation of Cr-rich precipitates were traced by analyzing the experimental atomic concentrations and chemical shifts with respect to annealing time, Cr content, and kinetic energy of the exited electron.

Mutually Exclusive Roles of SHARPIN in Integrin Inactivation and NF-κB Signaling
SHANK-associated RH domain interactor (SHARPIN) inhibits integrins through interaction with the integrin α-subunit. In addition, SHARPIN enhances nuclear factor-kappaB (NF-κB) activity as a component of the linear ubiquitin chain assembly complex (LUBAC). However, it is currently unclear how regulation of these seemingly different roles is coordinated. Here, we show that SHARPIN binds integrin and LUBAC in a mutually exclusive manner. We map the integrin binding site on SHARPIN to the ubiquitin-like (UBL) domain, the same domain implicated in SHARPIN interaction with LUBAC component RNF31 (ring finger protein 31), and identify two SHARPIN residues (V267, L276) required for both integrin and RNF31 regulation. Accordingly, the integrin α-tail is capable of competing with RNF31 for SHARPIN binding.
in vitro. Importantly, the full SHARPIN RNF31-binding site contains residues (F263A/I272A) that are dispensable for SHARPIN-integrin interaction. Importantly, disrupting SHARPIN interaction with integrin or RNF31 abolishes SHARPIN-mediated regulation of integrin or NF-κB activity, respectively. Altogether these data suggest that the roles of SHARPIN in inhibiting integrin activity and supporting linear ubiquitination are (molecularly) distinct.

**Self-subdiffusion in solutions of star-shaped crowders: non-monotonic effects of inter-particle interactions**

We examine by extensive computer simulations the self-diffusion of anisotropic star-like particles in crowded two-dimensional solutions. We investigate the implications of the area coverage fraction ϕ of the crowders and the crowder-crowder adhesion properties on the regime of transient anomalous diffusion. We systematically compute the mean squared displacement (MSD) of the particles, their time averaged MSD, and the effective diffusion coefficient. The diffusion is ergodic in the limit of long traces, such that the mean time averaged MSD converges towards the ensemble averaged MSD, and features a small residual amplitude spread of the time averaged MSD from individual trajectories. At intermediate time scales, we quantify the anomalous diffusion in the system. Also, we show that the translational-but not rotational-diffusivity of the particles D is a nonmonotonic function of the attraction strength between them. Both diffusion coefficients decrease as the power law D(ϕ) similar to (1 - ϕ/ϕ*)(2 ... 2.4) with the area fraction ϕ occupied by the crowders and the critical value ϕ*. Our results might be applicable to rationalising the experimental observations of non-Brownian diffusion for a number of standard macromolecular crowders used in vitro to mimic the cytoplasmic conditions of living cells.
Digital image correlation method in hydro turbine shaft torque and vibration monitoring

General information
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Ministry of Education publication type: D3 Professional conference proceedings
Organisations: Department of Mechanical Engineering and Industrial Systems, Research group: Kokeellinen
virtaustekniikka, Research area: Applied Mechanics, Department of Materials Science, Research group: Tribology and Machine Elements, Fortum Power and Heat Oy
Authors: Saarenrinne, P., Miettinen, J., Ylönen, M., Kokko, V.
Number of pages: 8
Publication date: 27 Oct 2015
Distributed-order diffusion equations and multifractality: Models and solutions

We study distributed-order time fractional diffusion equations characterized by multifractal memory kernels, in contrast to the simple power-law kernel of common time fractional diffusion equations. Based on the physical approach to anomalous diffusion provided by the seminal Scher-Montroll-Weiss continuous time random walk, we analyze both natural and modified-form distributed-order time fractional diffusion equations and compare the two approaches. The mean squared displacement is obtained and its limiting behavior analyzed. We derive the connection between the Wiener process, described by the conventional Langevin equation and the dynamics encoded by the distributed-order time fractional diffusion equation in terms of a generalized subordination of time. A detailed analysis of the multifractal properties of distributed-order diffusion equations is provided.

General information

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Radiat Safety Directorate, Univ Potsdam, University of Potsdam, Inst Phys & Astron, Univ Manchester, University of Manchester, Sch Math, Max Planck Inst Phys Komplexer Syst, Max Planck Society, Humboldt Univ, Humboldt University of Berlin, Inst Phys
Authors: Sandev, T., Chechkin, A. V., Korabel, N., Kantz, H., Sokolov, I. M., Metzler, R.
Keywords: (TIME RANDOM-WALKS, FOKKER-PLANCK EQUATION, GENERALIZED LANGEVIN EQUATION, MITTAG-LEFFLER FUNCTIONS, FRACTIONAL DIFFUSION, ANOMALOUS DIFFUSION, LEVY FLIGHTS, MASTER-EQUATIONS, KINETIC-THEORY, RELAXATION)
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Peer-reviewed: Yes

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Scopus rating (2016): 0.993 0.896
Publication Forum (2016): 1
Scopus rating (2015): 1.047 0.978
Publication Forum (2015): 1
Scopus rating (2014): 1.22 1.123
Web of Science (2014): 2.288 2.269 8.5 0.595 0.16687 0.859
Publication Forum (2014): 2
Scopus rating (2013): 1.311 1.239
Publication Forum (2013): 2
Scopus rating (2012): 1.42 1.226
Publication Forum (2012): 2
Scopus rating (2011): 1.485 1.225
Scopus rating (2010): 1.69 1.215
Scopus rating (2009): 1.694 1.259
Scopus rating (2008): 1.96 1.314
Quantifying the non-ergodicity of scaled Brownian motion

We examine the non-ergodic properties of scaled Brownian motion (SBM), a non-stationary stochastic process with a time dependent diffusivity of the form $D(t) \approx t^{\alpha - 1}$. We compute the ergodicity breaking parameter EB in the entire range of scaling exponents $\alpha$, both analytically and via extensive computer simulations of the stochastic Langevin equation. We demonstrate that in the limit of long trajectory lengths $T$ and short lag times $\Delta$ the EB parameter as function of the scaling exponent $\alpha$ has no divergence at $\alpha = 1/2$ and present the asymptotes for EB in different limits. We generalize the analytical and simulations results for the time averaged and ergodic properties of SBM in the presence of ageing, that is, when the observation of the system starts only a finite time span after its initiation. The approach developed here for the calculation of the higher time averaged moments of the particle displacement can be applied to derive the ergodic properties of other stochastic processes such as fractional Brownian motion.

General information

State: Published

Ministry of Education publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, Akhiezer Institute for Theoretical Physics, Kharkov Institute of Physics and Technology, Institute for Physics AndAstronomy, Humboldt-Universität zu Berlin, Shahid Beheshti University

Authors: Safdari, H., Cherstvy, A. G., Chechkin, A. V., Thiel, F., Sokolov, I. M., Metzler, R.

Keywords: (ageing, anomalous diffusion, scaled Brownian motion)

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Peer-reviewed: Yes

ASJC Scopus subject areas: Mathematical Physics, Physics and Astronomy(all), Statistical and Nonlinear Physics, Modelling and Simulation, Statistics and Probability

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Scopus rating (2016): 0.879 0.868
Publication Forum (2016): 1
Scopus rating (2015): 0.921 0.963
Web of Science (2015): 1.933 1.591 9.7 0.625 0.04241 0.711
Publication Forum (2015): 1
Scopus rating (2014): 0.92 0.918
Web of Science (2014): 1.583 1.476 9.3 0.615 0.05048 0.714
Publication Forum (2014): 2
Scopus rating (2013): 0.926 1.002
Publication Forum (2013): 2
Scopus rating (2012): 1.016 1.05
Publication Forum (2012): 2
Local oscillation of the boundary layer over the surface of swimming rainbow trout: implications for active drag reduction

The boundary layers of swimming rainbow trout, Oncorhynchus mykiss, were measured by the Particle Image Velocimetry (PIV) technique at a Reynolds number of 4×10^5. The flow velocity profile over the fish surface in a particular phase of undulatory motion had characteristics that were similar to the empirically-observed limit to drag reduction that was caused by adding high molecular weight polymers to wall-bounded turbulent flows, the so-called Virk’s asymptote. The rms velocity fluctuation in the stream-wise component (u rms+) in the reduced-drag flow regime increased with increasing drag reduction as consistently observed in the polymer-induced drag reducing flow. The distribution of the Reynolds stress suggested that turbulence makes a major contribution to the skin friction of rainbow trout that were swimming at the observed swimming speed (1 body-length s−1). The distribution of the turbulent kinetic energy (TKE) and the rate of TKE dissipation suggested that the fish surface that is moving in the direction of the free-stream flow can facilitate to retain the dilution rate of the mucus concentration at a certain level within the boundary layer. This causes more TKE to be gained from large scale eddies than can be dissipated into smaller scales.

Two-step semiclassical model for strong-field ionization with interference and multielectron polarization effects

We present a semiclassical model for above-threshold ionization with the inclusion of the Stark shift of the initial bound state, the Coulomb potential, and a polarization induced dipole potential capable to describe quantum interference. The model will be used to investigate the imprints of polarization effects in the interference structure of electron momentum distributions.
Building synthetic sterols computationally: unlocking the secrets of evolution?
Cholesterol is vital in regulating the physical properties of animal cell membranes. While it remains unclear what renders cholesterol so unique, it is known that other sterols are less capable in modulating membrane properties, and there are membrane proteins whose function is dependent on cholesterol. Practical applications of cholesterol include its use in liposomes in drug delivery and cosmetics, cholesterol-based detergents in membrane protein crystallography, its fluorescent analogs in studies of cholesterol transport in cells and tissues, etc. Clearly, in spite of their difficult synthesis, producing the synthetic analogs of cholesterol is of great commercial and scientific interest. In this article, we discuss how synthetic sterols non-existent in nature can be used to elucidate the roles of cholesterol's structural elements. To this end, we discuss recent atomistic molecular dynamics simulation studies that have predicted new synthetic sterols with properties comparable to those of cholesterol. We also discuss more recent experimental studies that have vindicated these predictions. The paper highlights the strength of computational simulations in making predictions for synthetic biology, thereby guiding experiments.
Parity-time-symmetric solitons in trapped Bose-Einstein condensates and the influence of varying complex potentials: A variational approach

Dynamics and properties of nonlinear matter waves in a trapped BEC subject to a PT-symmetric linear potential, with the trap in the form of a super-Gaussian potential, are investigated via a variational approach accounting for the complex nature of the soliton. In the process, we address how the shape of the imaginary part of the potential, that is, a gain-loss mechanism, affects the self-localization and the stability of the condensate. Variational results are found to be in good agreement with full numerical simulations for predicting the shape, width, and chemical potential of the condensate until the PT breaking point. Variational computation also predicts the existence of solitary solution only above a threshold in the particle number as the gain-loss is increased, in agreement with numerical simulations.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research group: Nonlinear Optics, Frontier Photonics, Universidade do Porto, Univ Roma Tre, Roma Tre University, Dept Elect Engn, NooEL, Cochin University of Science and Technology, Centro de Física Do Porto
Authors: Devassy, L., Jisha, C. P., Alberucci, A., Kuriakose, V. C.
Number of pages: 12
Publication date: 19 Aug 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability

Publication information
Journal: Physical Review E
Volume: 92
Issue number: 2
Article number: 022914
ISSN (Print): 1539-3755
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.993 0.896
Publication Forum (2016): 1
Scopus rating (2015): 1.047 0.978
Publication Forum (2015): 1
Scopus rating (2014): 1.22 1.123
Web of Science (2014): 2.288 2.269 8.5 0.595 0.16687 0.859
Publication Forum (2014): 2
Scopus rating (2013): 1.311 1.239
Publication Forum (2013): 2
Scopus rating (2012): 1.42 1.226
Publication Forum (2012): 2
Scopus rating (2011): 1.485 1.225
Scopus rating (2010): 1.69 1.215
Scopus rating (2009): 1.694 1.259
Scopus rating (2008): 1.96 1.314
Scopus rating (2007): 1.926 1.332
Caustics and rogue waves in an optical sea
There are many examples in physics of systems showing rogue wave behaviour, the generation of high amplitude events at low probability. Although initially studied in oceanography, rogue waves have now been seen in many other domains, with particular recent interest in optics. Although most studies in optics have focussed on how nonlinearity can drive rogue wave emergence, purely linear effects have also been shown to induce extreme wave amplitudes. In this paper, we report a detailed experimental study of linear rogue waves in an optical system, using a spatial light modulator to impose random phase structure on a coherent optical field. After free space propagation, different random intensity patterns are generated, including partially-developed speckle, a broadband caustic network, and an intermediate pattern with characteristics of both speckle and caustic structures. Intensity peaks satisfying statistical criteria for rogue waves are seen especially in the case of the caustic network, and are associated with broader spatial spectra. In addition, the electric field statistics of the intermediate pattern shows properties of an optical sea with near-Gaussian statistics in elevation amplitude, and trough-to-crest statistics that are near-Rayleigh distributed but with an extended tail where a number of rogue wave events are observed.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research group: Nonlinear Fiber Optics, Frontier Photonics, School of Mathematical Sciences, Institut FEMTO-ST, UMR 6174 CNRS-Université de Franche-Comté, University College Dublin
Authors: Mathis, A., Froehly, L., Toenger, S., Dias, F., Genty, G., Dudley, J. M.
Publication date: 6 Aug 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: General

Publication information
Journal: Scientific Reports
Volume: 5
Article number: 12822
ISSN (Print): 2045-2322
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.625 1.401
Publication Forum (2016): 2
Scopus rating (2015): 2.057 1.684
Web of Science (2015): 5.228 5.525 2.1 0.559 0.209 1.865
Publication Forum (2015): 2
Scopus rating (2014): 2.103 1.544
Web of Science (2014): 5.578 5.597 1.7 0.722 0.11476 2.075
Publication Forum (2014): 1
Scopus rating (2013): 1.886 1.51
Publication Forum (2013): 1
Scopus rating (2012): 1.458 0.896
Publication Forum (2012): 1
Effect of Phosphatidic Acid on Biomembrane: Experimental and Molecular Dynamics Simulations Study

We consider the impact of phosphatidic acid (namely, 1,2-dioleoyl-sn-glycero-3-phosphate, DOPA) on the properties of a zwitterionic (1,2-dipalmitoyl-sn-glycero-3-phosphocholine, DPPC) bilayer used as a model system for protein-free cell membranes. For this purpose, experimental measurements were performed using differential scanning calorimetry and the Langmuir monolayer technique at physiological pH. Moreover, atomistic-scale molecular dynamics (MD) simulations were performed to gain information on the mixed bilayer's molecular organization. The results of the monolayer studies clearly showed that the DPPC/DOPA mixtures are nonideal and the interactions between lipid species change from attractive, at low contents of DOPA, to repulsive, at higher contents of that component. In accordance with these results, the MD simulations demonstrated that both monoanionic and dianionic forms of DOPA have an ordering and condensing effect on the mixed bilayer at low concentrations. For the DOPA monoanions, this is the result of both (i) strong electrostatic interactions between the negatively charged oxygen of DOPA and the positively charged choline groups of DPPC and (ii) conformational changes of the lipid acyl chains, leading to their tight packing according to the so-called umbrella model, in which large headgroups of DPPC shield the hydrophobic part of DOPA (the conical shape lipid) from contact with water. In the case of the DOPA dianions, cation-mediated clustering was observed. Our results provide a detailed molecular-level description of the lipid organization inside the mixed zwitterionic/PA membranes, which is fully supported by the experimental data.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Computational Science X (CompX), Jagiellonian University, Faculty of Chemistry
Authors: Kwolek, U., Kulig, W., Wydro, P., Nowakowska, M., Róg, T., Kepczynski, M.
Number of pages: 10
Pages: 10042-10051
Publication date: 6 Aug 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

Publication Information
Journal: Journal of Physical Chemistry Part B
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ISSN (Print): 1520-6106
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.348 1.02
Publication Forum (2016): 1
Scopus rating (2015): 1.367 1.096
Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
Publication Forum (2015): 1
Scopus rating (2014): 1.44 1.14
Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
Publication Forum (2014): 3
Scopus rating (2013): 1.494 1.2
Publication Forum (2013): 3
Scopus rating (2012): 1.92 1.251
Publication Forum (2012): 3
Scopus rating (2011): 1.78 1.226
Scopus rating (2010): 1.849 1.214
Scopus rating (2009): 2.232 1.349
Scopus rating (2008): 2.543 1.381
Diffusion and Fokker-Planck-Smoluchowski equations with generalized memory kernel

We consider anomalous stochastic processes based on the renewal continuous time random walk model with different forms for the probability density of waiting times between individual jumps. In the corresponding continuum limit we derive the generalized diffusion and Fokker-Planck-Smoluchowski equations with the corresponding memory kernels. We calculate the qth order moments in the unbiased and biased cases, and demonstrate that the generalized Einstein relation for the considered dynamics remains valid. The relaxation of modes in the case of an external harmonic potential and the convergence of the mean squared displacement to the thermal plateau are analyzed.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, Radiation Safety Directorate, Akhiezer Institute for Theoretical Physics
Authors: Sandev, T., Chechkin, A., Kantz, H., Metzler, R.
Keywords: (anomalous diffusion, continuous time random walk (CTRW), Fokker-Planck-Smoluchowski equation, Mittag-Leffler functions, multi-scaling)
Number of pages: 33
Pages: 1006-1038
Publication date: 1 Aug 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Analysis, Applied Mathematics

Publication information
Journal: Fractional Calculus and Applied Analysis
Volume: 18
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Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.372 1.492
Publication Forum (2016): 1
Scopus rating (2015): 1.449 1.492
Publication Forum (2015): 1
Scopus rating (2014): 1.364 1.611
Publication Forum (2014): 1
Scopus rating (2013): 2.075 2.22
Publication Forum (2013): 1
Scopus rating (2012): 1.045 1.026
Publication Forum (2012): 1
Original language: English
DOIs:
10.1515/fca-2015-0059
Nonlinear Optical Properties of Fluorescent Dyes Allow for Accurate Determination of Their Molecular Orientations in Phospholipid Membranes

Several methods based on single- and two-photon fluorescence detected linear dichroism have recently been used to determine the orientational distributions of fluorescent dyes in lipid membranes. However, these determinations relied on simplified descriptions of nonlinear anisotropic properties of the dye molecules, using a transition dipole-moment-like vector instead of an absorptivity tensor. To investigate the validity of the vector approximation, we have now carried out a combination of computer simulations and polarization microscopy experiments on two representative fluorescent dyes (DiI and F2N12S) embedded in aqueous phosphatidylcholine bilayers. Our results indicate that a simplified vector-like treatment of the two-photon transition tensor is applicable for molecular geometries sampled in the membrane at ambient conditions. Furthermore, our results allow evaluation of several distinct polarization microscopy techniques. In combination, our results point to a robust and accurate experimental and computational treatment of orientational distributions of DiI, F2N12S, and related dyes (including Cy3, Cy5, and others), with implications to monitoring physiologically relevant processes in cellular membranes in a novel way.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Lawrence Berkeley National Laboratory, Department of Cybernetics, Faculty of Applied Sciences, University of West Bohemia, Institute of Nanobiology and Structural Biology GCRC, V.v.i., Academy of Sciences of the Czech Republic, University of South Bohemia
Authors: Timr, Š., Brabec, J., Bondar, A., Ryba, T., Železný, M., Lazar, J., Jungwirth, P.
Number of pages: 11
Pages: 9706-9716
Publication date: 30 Jul 2015
Peer-reviewed: Yes
Early online date: 21 Jul 2015
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

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Journal: Journal of Physical Chemistry Part B
Volume: 119
Issue number: 30
ISSN (Print): 1520-6106
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.348 1.02
Publication Forum (2016): 1
Scopus rating (2015): 1.367 1.096
Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
Publication Forum (2015): 1
Scopus rating (2014): 1.44 1.14
Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
Publication Forum (2014): 3
Scopus rating (2013): 1.494 1.2
Publication Forum (2013): 3
Scopus rating (2012): 1.92 1.251
Publication Forum (2012): 3
Scopus rating (2011): 1.78 1.226
Scopus rating (2010): 1.849 1.214
Scopus rating (2009): 2.232 1.349
Scopus rating (2008): 2.543 1.381
Scopus rating (2007): 2.346 1.282
Scopus rating (2006): 2.369 1.415
Data-Driven Approach for Analysis of Performance Indices in Mobile Work Machines

This paper presents a data-driven approach for the analysis of performance indices in mobile work machines. Performance analysis and optimisation of mobile work machines has become increasingly important in recent years. The mobile work machine optimisation is performed based on performance measurements. One of the most interesting and potential approach for improving the quality of the performance analysis is the utilisation of Big Data and data-driven analysis methods, such as machine learning. This study utilises a machine learning algorithm, Classification and Regression Trees (CART), in the performance analysis of the mobile work machines. The most significant benefit of the presented method is that it provides a statistical reference of the machine performance for the operators. The method enables operators to compare performance against reference fleet of machines working in similar operating conditions. This feature can lead to more informative and reliable interpretations and analysis of the performance values. The results of this paper demonstrate how the presented method was used to analyse the performance of a mobile work machine fleet.

Ageing first passage time density in continuous time random walks and quenched energy landscapes

We study the first passage dynamics of an ageing stochastic process in the continuous time random walk (CTRW) framework. In such CTRW processes the test particle performs a random walk, in which successive steps are separated by random waiting times distributed in terms of the waiting time probability density function \( \varphi(t) \approx t^{-\alpha} \) \((0 \leq \alpha \leq 2)\). An ageing stochastic process is defined by the explicit dependence of its dynamic quantities on the ageing time \( t_{a} \), the time elapsed between its preparation and the start of the observation. Subdiffusive ageing CTRWs with \(0 < \alpha < 1\) describe systems such as charge carriers in amorphous semiconductors, tracer dispersion in geological and biological systems, or the dynamics of blinking quantum dots. We derive the exact forms of the first passage time density for an ageing subdiffusive CTRW in the semi-infinite, confined, and biased case, finding different scaling regimes for weakly, intermediately, and strongly aged systems: these regimes, with different scaling laws, are also found when the scaling exponent is in the range \( 1 < \alpha < 2\), for sufficiently long \( t_{a} \). We compare our results with the ageing motion of a test particle in a quenched energy landscape. We test our theoretical results in the quenched landscape against simulations: only when the bias is strong enough, the correlations from returning to previously visited sites become
insignificant and the results approach the ageing CTRW results. With small bias or without bias, the ageing effects disappear and a change in the exponent compared to the case of a completely annealed landscape can be found, reflecting the build-up of correlations in the quenched landscape.

**General information**

State: Published

Ministry of Education publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, National Institute of Chemistry Ljubljana

Authors: Krüsemann, H., Godec, A., Metzler, R.

Keywords: (anomalous diffusion, first passage, random walks)

Publication date: 17 Jul 2015

Peer-reviewed: Yes

ASJC Scopus subject areas: Mathematical Physics, Physics and Astronomy(all), Statistical and Nonlinear Physics, Modelling and Simulation, Statistics and Probability

**Publication information**

Journal: Journal of Physics A: Mathematical and Theoretical

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Article number: 285001

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Ratings:

Publication Forum (2017): 1
Scopus rating (2016): 0.879 0.868
Publication Forum (2016): 1
Scopus rating (2015): 0.921 0.963
Web of Science (2015): 1.933 1.591 9.7 0.625 0.04241 0.711
Publication Forum (2015): 1
Scopus rating (2014): 0.92 0.918
Web of Science (2014): 1.583 1.476 9.3 0.615 0.05048 0.714
Publication Forum (2014): 2
Scopus rating (2013): 0.926 1.002
Publication Forum (2013): 2
Scopus rating (2012): 1.016 1.05
Publication Forum (2012): 2
Scopus rating (2011): 0.934 0.946
Scopus rating (2010): 1.056 1.037
Scopus rating (2009): 1.075 1.001
Scopus rating (2008): 1.136 1.071
Scopus rating (2007): 1.151 1.152
Scopus rating (2006): 0.97 1.038
Scopus rating (2005): 0.996 0.981
Scopus rating (2004): 0.98 0.939
Scopus rating (2003): 0.841 0.931
Scopus rating (2002): 0.828 0.988
Scopus rating (2001): 0.775 1.005
Scopus rating (2000): 0.938 0.856
Scopus rating (1999): 1.086 0.868

Original language: English

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10.1088/1751-8113/48/28/285001

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Source: Scopus

Source-ID: 84937118398

Research output: Scientific - peer-review › Article
Numerical Path Integral Approach to Quantum Dynamics and Stationary Quantum States

Applicability of Feynman path integral approach to numerical simulations of quantum dynamics of an electron in real time domain is examined. Coherent quantum dynamics is demonstrated with one dimensional test cases (quantum dot models) and performance of the Trotter kernel as compared with the exact kernels is tested. Also, a novel approach for finding the ground state and other stationary states is presented. This is based on the incoherent propagation in real time. For both approaches the Monte Carlo grid and sampling are tested and compared with regular grids and sampling. We assess the numerical prerequisites for all of the above.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research group: Electronic Structure Theory
Authors: Ruokosenmäki, I., Rantala, T. T.
Keywords: (incoherent propagation, Path integral, quantum dynamics, real time domain, stationary states)
Number of pages: 13
Pages: 91-103
Publication date: 3 Jul 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Physics and Astronomy (miscellaneous)

Publication information
Journal: Communications in Computational Physics
Volume: 18
Issue number: 1
ISSN (Print): 1815-2406
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.97 0.892
Publication Forum (2016): 1
Scopus rating (2015): 1.096 1.18
Web of Science (2015): 1.778 1.752 4.4 0.319 0.00812 0.854
Publication Forum (2015): 1
Scopus rating (2014): 1.299 1.25
Web of Science (2014): 1.943 1.913 3.9 0.565 0.00935 0.946
Publication Forum (2014): 1
Scopus rating (2013): 1.301 1.09
Publication Forum (2013): 1
Scopus rating (2012): 1.25 1.351
Publication Forum (2012): 1
Scopus rating (2011): 1.048 1.376
Scopus rating (2010): 1.272 1.427
Scopus rating (2008): 1.285 1.25
Original language: English
DOI: 10.4208/cicp.180914.161214a
Links:
http://www.scopus.com/inward/record.url?scp=84937030531&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source-ID: 84937030531
Research output: Scientific - peer-review › Article

Signal focusing through active transport

The accuracy of molecular signaling in biological cells and novel diagnostic devices is ultimately limited by the counting noise floor imposed by the thermal diffusion. Motivated by the fact that messenger RNA and vesicle-engulfed signaling molecules transiently bind to molecular motors and are actively transported in biological cells, we show here that the random active delivery of signaling particles to within a typical diffusion distance to the receptor generically reduces the correlation time of the counting noise. Considering a variety of signaling particle sizes from mRNA to vesicles and cell sizes from prokaryotic to eukaryotic cells, we show that the conditions for active focusing - faster and more precise signaling - are indeed compatible with observations in living cells. Our results improve the understanding of molecular cellular signaling and novel diagnostic devices.
Cholesterol under oxidative stress: How lipid membranes sense oxidation as cholesterol is being replaced by oxysterols

The behavior of oxysterols in phospholipid membranes and their effects on membrane properties were investigated by means of dynamic light scattering, fluorescence spectroscopy, NMR, and extensive atomistic simulations. Two families of oxysterols were scrutinized - tail-oxidized sterols, which are mostly produced by enzymatic processes, and ring-oxidized sterols, formed mostly via reactions with free radicals. The former family of sterols was found to behave similar to cholesterol in terms of molecular orientation, roughly parallel to the bilayer normal, leading to increasing membrane stiffness and suppression of its membrane permeability. In contrast, ring-oxidized sterols behave quantitatively differently from cholesterol. They acquire tilted orientations and therefore disrupt the bilayer structure with potential implications for
signaling and other biochemical processes in the membranes.

**General information**

State: Published

Ministry of Education publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Oulu, Tallinn Technical University, Institute of Chemistry, University of Southern Denmark, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Department of Physics and Chemistry, Weill Cornell Medical College, Fritz Haber Research Center, Hebrew University of Jerusalem

Authors: Kulig, W., Olzyńska, A., Jurkiewicz, P., Kantola, A. M., Komulainen, S., Manna, M., Pourmousa, M., Vazdar, M., Cwiklik, L., Rog, T., Khelashvili, G., Harries, D., Telkki, V. V., Hof, M., Vattulainen, I., Jungwirth, P.

Keywords: (Phospholipid bilayers, Oxysterols, Molecular dynamics simulations, DPH anisotropy, NMR measurements, Laurdan fluorescence, Liposomes, Tilt modulus, FLUORESCENCE SOLVENT RELAXATION, MOLECULAR-DYNAMICS METHOD, MODEL MEMBRANES, FOURIER TRANSFORMATION, POTENTIAL FUNCTIONS, SOLVATION DYNAMICS, BENDING RIGIDITY, ORDER PARAMETERS, BILAYERS, PROTEINS)

Number of pages: 12

Publication date: 1 Jul 2015

Peer-reviewed: Yes

ASJC Scopus subject areas: Biochemistry, Physiology (medical)

**Publication information**

Journal: Free Radical Biology and Medicine

Volume: 84

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Publication Forum (2017): 1
Scopus rating (2016): 2.276 1.529
Publication Forum (2016): 1
Scopus rating (2015): 2.511 1.627
Web of Science (2015): 5.784 5.982 8.6 1.167 0.04786 1.568
Publication Forum (2015): 1
Scopus rating (2014): 2.458 1.664
Web of Science (2014): 5.736 5.855 8.4 1.147 0.04814 1.5
Publication Forum (2014): 2
Scopus rating (2013): 2.218 1.691
Publication Forum (2013): 2
Scopus rating (2012): 2.099 1.67
Publication Forum (2012): 2
Scopus rating (2011): 2.172 1.734
Scopus rating (2010): 2.312 1.68
Scopus rating (2009): 2.191 1.524
Scopus rating (2008): 2.204 1.463
Scopus rating (2007): 2.167 1.56
Scopus rating (2006): 2.169 1.632
Scopus rating (2005): 2.3 1.642
Scopus rating (2004): 2.307 1.778
Scopus rating (2003): 2.377 1.812
Scopus rating (2002): 2.137 1.794
Scopus rating (2001): 1.831 1.598
Scopus rating (2000): 1.582 1.499
Scopus rating (1999): 1.878 1.723

Original language: English

DOIs:

10.1016/j.freeradbiomed.2015.03.006

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http://www.scopus.com/inward/record.url?scp=84928530055&partnerID=8YFLLogxK (Link to publication in Scopus)

Source: WOS

Source-ID: 000355896500004
Holographic entanglement entropy in 2D holographic superconductor via AdS3/CFT2

The aim of the present letter is to find the holographic entanglement entropy (HEE) in 2D holographic superconductors (HSC). Indeed, it is possible to compute the exact form of this entropy due to an advantage of approximate solutions inside normal and superconducting phases with backreactions. By making the UV and IR limits applied to the integrals, an approximate expression for HEE is obtained. In case the software cannot calculate minimal surface integrals analytically, it offers the possibility to proceed with a numerical evaluation of the corresponding terms. We'll understand how the area formula incorporates the structure of the domain wall approximation. We see that HEE changes linearly with belt angle. It's due to the extensivity of this type of entropy and the emergent of an entropic force. We find that the wider belt angle corresponds to a larger holographic surface. Another remarkable observation is that no "confinement/deconfinement" phase transition point exists in our 2D dual field theory. Furthermore, we observe that the slope of the HEE with respect to the temperature $dS/dT$ decreases, thanks to the emergence extra degree of freedom(s) in low temperature system. A first order phase transition is detected near the critical point.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Eurasian International Center for Theoretical Physics, Centre for Optical and Electromagnetic Research, Dept. of General and Theoretical Physics, Eurasian National University, COMSATS Institute of Information Technology, State Key Lab of Modern Optical Instrumentation, Department of Optical Engineering, Zhejiang University
Authors: Momeni, D., Gholizade, H., Raza, M., Myrzakulov, R.
Number of pages: 9
Pages: 417-425
Publication date: 1 Jul 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Nuclear and High Energy Physics

Publication information
Journal: Physics Letters B
Volume: 747
ISSN (Print): 0370-2693
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 3.309 2.265
Publication Forum (2016): 2
Scopus rating (2015): 3.239 2.112
Web of Science (2015): 4.787 3.966 >10.0 1.747 0.09563 1.489
Publication Forum (2015): 2
Scopus rating (2014): 3.538 1.988
Web of Science (2014): 6.131 4.08 >10.0 2.104 0.1051 1.52
Publication Forum (2014): 2
Scopus rating (2013): 3.707 2.073
Publication Forum (2013): 2
Scopus rating (2012): 3.37 1.677
Publication Forum (2012): 2
Scopus rating (2011): 3.02 1.569
Scopus rating (2010): 3.067 1.433
Scopus rating (2009): 2.862 1.557
Scopus rating (2008): 2.826 1.326
Scopus rating (2007): 3.003 1.505
Scopus rating (2006): 3.096 1.376
Scopus rating (2005): 2.713 1.399
Scopus rating (2004): 2.592 1.293
Scopus rating (2003): 2.931 1.229
Scopus rating (2002): 2.705 1.214
Scopus rating (2001): 3.021 1.33
Scopus rating (2000): 3.31 1.395
How To Minimize Artifacts in Atomistic Simulations of Membrane Proteins, Whose Crystal Structure Is Heavily Engineered: beta(2)-Adrenergic Receptor in the Spotlight

Atomistic molecular dynamics (MD) simulations are used extensively to elucidate membrane protein properties. These simulations are based on three-dimensional protein structures that in turn are often based on crystallography. The protein structures resolved in crystallographic studies typically do not correspond to pristine proteins, however. Instead the crystallized proteins are commonly engineered, including structural modifications (mutations, replacement of protein sequences by antibodies, bound ligands, etc.) whose impact on protein structure and dynamics is largely unknown. Here we explore this issue through atomistic MD simulations (,5 its in total), focusing on the beta(2)-adrenergic receptor (beta(2)AR) that is one of the most studied members of the G-protein coupled receptor superfamily. Starting from an inactive-state crystal structure beta(2)AR, we remove the many modifications in beta(2)AR systematically one at a time, in six consecutive steps. After each step, we equilibrate the system and simulate it quite extensively. The results of this step-by-step approach highlight that the structural modifications used in crystallization can affect ligand and G-protein binding sites, packing at the transmembrane-helix interface region, and the dynamics of connecting loops in beta(2)AR. When the results of the systematic step-by-step approach are compared to an all-at-once technique where all modifications done on beta(2)AR are removed instantaneously at the same time, it turns out that the step-by-step method provides results that are superior in terms of maintaining protein structural stability. The results provide compelling evidence that for membrane proteins whose 3D structure is based on structural engineering, the preparation of protein structure for atomistic MD simulations is a delicate and sensitive process. The results show that most valid results are found when the structural modifications are reverted slowly, one at a time.
Membrane targeting of the yeast exocyst complex

The exocytosis is a process of fusion of secretory vesicles with the plasma membrane, which plays a prominent role in many crucial cellular processes, e.g. secretion of neurotransmitters, cytokinesis or yeast budding. Prior to the SNARE-mediated fusion, the initial contact of secretory vesicle with the target membrane is mediated by an evolutionarily conserved vesicle tethering protein complex, the exocyst. In all eukaryotic cells, the exocyst is composed of eight subunits - Sec5, Sec6, Sec8, Sec10, Sec15, Exo84 and two membrane-targeting landmark subunits Sec3 and Exo70, which have been described to directly interact with phosphatidylinositol (4,5)-bisphosphate (PIP2) of the plasma membrane. In this work, we utilized coarse-grained molecular dynamics simulations to elucidate structural details of the interaction of yeast Sec3p and Exo70p with lipid bilayers containing PIP2. We found that PIP2 is coordinated by the positively charged pocket of N-terminal part of Sec3p, which folds into unique Pleckstrin homology domain. Conversely, Exo70p interacts with the lipid bilayer by several binding sites distributed along the structure of this exocyst subunit. Moreover, we observed that the interaction of Exo70p with the membrane causes clustering of PIP2 in the adjacent leaflet. We further revealed that PIP2 is required for the correct positioning of small GTPase Rho1p, a direct Sec3p interactor, prior to the formation of the functional Rho1p-exocyst-membrane assembly. Our results show the critical importance of the plasma membrane pool of PIP2 for the exocyst function and suggest that specific interaction with acidic phospholipids represents an ancestral mechanism for the exocyst regulation. (C) 2015 Elsevier B.V. All rights reserved.
Superdiffusion dominates intracellular particle motion in the supercrowded cytoplasm of pathogenic Acanthamoeba castellanii

Acanthamoebae are free-living protists and human pathogens, whose cellular functions and pathogenicity strongly depend on the transport of intracellular vesicles and granules through the cytosol. Using high-speed live cell imaging in combination with single-particle tracking analysis, we show here that the motion of endogenous intracellular particles in the size range from a few hundred nanometers to several micrometers in Acanthamoeba castellanii is strongly superdiffusive and influenced by cell locomotion, cytoskeletal elements, and myosin II. We demonstrate that cell locomotion significantly contributes to intracellular particle motion, but is clearly not the only origin of superdiffusivity. By analyzing the contribution of microtubules, actin, and myosin II motors we show that myosin II is a major driving force of intracellular motion in A. castellanii. The cytoplasm of A. castellanii is supercrowded with intracellular vesicles and granules, such that significant intracellular motion can only be achieved by actively driven motion, while purely thermally driven diffusion is negligible.
Ultraslow scaled Brownian motion

We define and study in detail ultraslow scaled Brownian motion (USBM) characterized by a time dependent diffusion coefficient of the form $D(t) \sim \frac{1}{t}$. For unconfined motion the mean squared displacement (MSD) of USBM exhibits an ultraslow, logarithmic growth as function of time, in contrast to the conventional scaled Brownian motion. In a harmonic potential the MSD of USBM does not saturate but asymptotically decays inverse-proportionally to time, reflecting the highly non-stationary character of the process. We show that the process is weakly non-ergodic in the sense that the time averaged MSD does not converge to the regular MSD even at long times, and for unconfined motion combines a linear lag time dependence with a logarithmic term. The weakly non-ergodic behaviour is quantified in terms of the ergodicity breaking parameter. The USBM process is also shown to be ageing: observables of the system depend on the time gap between initiation of the test particle and start of the measurement of its motion. Our analytical results are shown to agree excellently with extensive computer simulations.
Effect of electron-phonon interaction on the formation of one-dimensional electronic states in coupled Cl vacancies

The formation of extended electron states in one-dimensional nanostructures is of key importance for the function of molecular electronic devices. Here, we study the effects of strong electron-phonon interaction on the formation of extended electronic states in intentionally created Cl vacancy pairs and chains in a NaCl bilayer on Cu(111). The interaction between the vacancies was tailored by fabricating vacancy pairs and chains of different orientation and separation with atomic precision using vertical manipulation. Small vacancy separations led to the formation of quantum-well-like vacancy states and localized interface states. By using scanning tunneling spectroscopy, we measured their energy splitting and broadening as a function of the intervacancy separation. Remarkably, the energy splitting between the vacancy states is enlarged by level repulsion resulting from the phonon dressing of the electronic states, as evidenced by theory.

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Authors: Schuler, B., Persson, M., Paavilainen, S., Pavlicek, N., Gross, L., Meyer, G., Repp, J.
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Investigation of an entropic stabilizer for the lattice-Boltzmann method

The lattice-Boltzmann (LB) method is commonly used for the simulation of fluid flows at the hydrodynamic level of description. Due to its kinetic theory origins, the standard LB schemes carry more degrees of freedom than strictly needed, e.g., for the approximation of solutions to the Navier-stokes equation. In particular, there is freedom in the details of the so-called collision operator. This aspect was recently utilized when an entropic stabilizer, based on the principle of maximizing local entropy, was proposed for the LB method [I. V. Karlin, F. Bösch, and S. S. Chikatamarla, Phys. Rev. E 90, 031302(R) (2014)]. The proposed stabilizer can be considered as an add-on or extension to basic LB schemes. Here the entropic stabilizer is investigated numerically using the perturbed double periodic shear layer flow as a benchmark case. The investigation is carried out by comparing numerical results obtained with six distinct LB schemes. The main observation is that the unbounded, and not explicitly controllable, relaxation time for the higher-order moments will directly influence the leading-order error terms. As a consequence, the order of accuracy and, in general, the numerical behavior of LB schemes are substantially altered. Hence, in addition to systematic numerical validation, more detailed theoretical analysis of the entropic stabilizer is still required in order to properly understand its properties.

General information

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Inverted critical adsorption of polyelectrolytes in confinement

What are the fundamental laws for the adsorption of charged polymers onto oppositely charged surfaces, for convex, planar, and concave geometries? This question is at the heart of surface coating applications, various complex formation phenomena, as well as in the context of cellular and viral biophysics. It has been a long-standing challenge in theoretical polymer physics; for realistic systems the quantitative understanding is however often achievable only by computer simulations. In this study, we present the findings of such extensive Monte-Carlo in silico experiments for polymer-surface adsorption in confined domains. We study the inverted critical adsorption of finite-length polyelectrolytes in three fundamental geometries: planar slit, cylindrical pore, and spherical cavity. The scaling relations extracted from simulations for the critical surface charge density $\sigma_{c}$ - defining the adsorption-desorption transition - are in excellent agreement with our analytical calculations based on the ground-state analysis of the Edwards equation. In particular, we confirm the magnitude and scaling of $\sigma_{c}$ for the concave interfaces versus the Debye screening length $1/\kappa$ and the extent of confinement $a$ for these three interfaces for small $ka$ values. For large $k$ the critical adsorption condition approaches the known planar limit. The transition between the two regimes takes place when the radius of surface curvature or half of the slit thickness $a$ is of the order of $1/\kappa$. We also rationalize how $\sigma_{c}$ dependence gets modified for semi-flexible versus flexible chains under external confinement. We examine the implications of the chain length for critical adsorption - the effect often hard to tackle theoretically - putting an emphasis on polymers inside attractive spherical cavities. The applications of our findings to some biological systems are discussed, for instance the adsorption of nucleic acids onto the inner surfaces of cylindrical and spherical viral capsids.
Myelin protein P2 is a fatty acid-binding structural component of the myelin sheath in the peripheral nervous system, and its function is related to its membrane binding capacity. Here, the link between P2 protein dynamics and structure and function was studied using elastic incoherent neutron scattering (EINS). The P38G mutation, at the hinge between the β barrel and the α-helical lid, increased the lipid stacking capacity of human P2 in vitro, and the mutated protein was also functional in cultured cells. The P38G mutation did not change the overall structure of the protein. For a deeper insight into P2 structure-function relationships, information on protein dynamics in the 10 ps to 1 ns time scale was obtained using EINS. Values of mean square displacements mainly from protein H atoms were extracted for wild-type P2 and the P38G mutant and compared. Our results show that at physiological temperatures, the P38G mutant is more dynamic than the wild-type P2 protein, especially on a slow 1-ns time scale. Molecular dynamics simulations confirmed the enhanced dynamics of the mutant variant, especially within the portal region in the presence of bound fatty acid. The increased softness of the hinge mutant of human myelin P2 protein is likely related to an enhanced flexibility of the portal region of this fatty acid-binding protein, as well as to its interactions with the lipid bilayer surface requiring conformational adaptations.
Tolman-Oppenheimer-Volkoff equations in nonlocal f(R) gravity

Nonlocal f(R) gravity was proposed as a powerful alternative to general relativity (GR). This theory has potentially adverse implications for infrared (IR) regime as well as ultraviolet (UV) early epochs. However, there are a lot of powerful features, making it really user-friendly. A scalar-tensor frame comprising two auxiliary scalar fields is used to reduce complex action. However, this is not the case for the modification complex which plays a distinct role in modified theories for gravity. In this work, we study the dynamics of a static, spherically symmetric object. The interior region of space-time had rapidly filled the perfect fluid. However, it is possible to derive a physically based model which relates interior metric to nonlocal f(R).

The Tolman-Oppenheimer-Volkoff (TOV) equations would be a set of first-order differential equations from which we can deduce all mathematical (physical) truths and derive all dynamical objects. This set of dynamical equations govern pressure $p$, density $\rho$, mass $m$ and auxiliary fields $\phi, \xi$. The full conditional solutions are evaluated and inverted numerically to obtain exact forms of the compact stars Her X-1, SAX J 1808.4-3658 and 4U 1820-30 for nonlocal Starobinsky model of $f(\rightarrow^{-1} R) = \rightarrow^{-1} R + \alpha(\rightarrow^{-1} R)^2$. The program solves the differential equations numerically using adaptive Gaussian quadrature. An ascription of correctness is supposed to be an empirical equation of state $P/P_{\text{c}} = a (1-e^{b\rho/\rho_{\text{c}}})$ for star which is informative in so far as it excludes an alternative nonlocal approach to compact star formation. This model is most suited for astrophysical observation.
PEGylated liposomes as carriers of hydrophobic porphyrins

Sterically stabilized liposomes (SSLs) (PEGylated liposomes) are applied as effective drug delivery vehicles. Understanding the interactions between hydrophobic compounds and PEGylated membranes is therefore important to
determine the effectiveness of PEGylated liposomes for delivery of drugs or other bioactive substances. In this study, we have combined fluorescence quenching analysis (FQA) experiments and all-atom molecular dynamics (MD) simulations to study the effect of membrane PEGylation on the location and orientation of 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin (p-THPP) that has been used in our study as a model hydrophobic compound. First, we consider the properties of p-THPP in the presence of different fluid phosphatidylcholine bilayers that we use as model systems for protein-free cell membranes. Next, we studied the interaction between PEGylated membranes and p-THPP. Our MD simulation results indicated that the arrangement of p-THPP within zwitterionic membranes is dependent on their free volume, and p-THPP solubilized in PEGylated liposomes is localized in two preferred positions: deep within the membrane (close to the center of the bilayer) and in the outer PEG corona (p-THPP molecules being wrapped with the polymer chains). Fluorescence quenching methods confirmed the results of atomistic MD simulations and showed two populations of p-THPP molecules as in MD simulations. Our results provide both an explanation for the experimental observation that PEGylation improves the drug-loading efficiency of membranes and also a more detailed molecular-level description of the interactions between porphyrins and lipid membranes.

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Authors: Dzieciuch, M., Rissanen, S., Szydłowska, N., Bunker, A., Kumorek, M., Jamróz, D., Vattulainen, I., Nowakowska, M., Róg, T., Kepczynski, M.
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Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
Publication Forum (2015): 1
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Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
Publication Forum (2014): 3
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Publication Forum (2013): 3
Scopus rating (2012): 1.92 1.251
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Scopus rating (2011): 1.78 1.226
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Scopus rating (2006): 2.369 1.415
Scopus rating (2005): 2.275 1.474
Scopus rating (2004): 2.148 1.511
Scopus rating (2003): 2.034 1.47
Scopus rating (2002): 2.118 1.496
Scopus rating (2001): 2.053 1.508
Scopus rating (2000): 2.145 1.527
Scopus rating (1999): 1.713 1.8
Fluctuations of Hi-Hat Timing and Dynamics in a Virtuoso Drum Track of a Popular Music Recording

Long-range correlated temporal fluctuations in the beats of musical rhythms are an inevitable consequence of human action. According to recent studies, such fluctuations also lead to a favored listening experience. The scaling laws of amplitude variations in rhythms, however, are widely unknown. Here we use highly sensitive onset detection and time series analysis to study the amplitude and temporal fluctuations of Jeff Porcaro's one-handed hi-hat pattern in "I Keep Forgettin'"—one of the most renowned 16th note patterns in modern drumming. We show that fluctuations of hi-hat amplitudes and interbeat intervals (times between hits) have clear long-range correlations and short-range anticorrelations separated by a characteristic time scale. In addition, we detect subtle features in Porcaro's drumming such as small drifts in the 16th note pulse and non-trivial periodic two-bar patterns in both hi-hat amplitudes and intervals. Through this investigation we introduce a step towards statistical studies of the 20th and 21st century music recordings in the framework of complex systems. Our analysis has direct applications to the development of drum machines and to drumming pedagogy.
Apolipoprotein A-I mimetic peptide 4F blocks sphingomyelinase-induced LDL aggregation

Lipolytic modification of LDL particles by SMase generates LDL aggregates with a strong affinity for human arterial proteoglycans and may so enhance LDL retention in the arterial wall. Here, we evaluated the effects of apoA-I mimetic peptide 4F on structural and functional properties of the SMase-modified LDL particles. LDL particles with and without 4F were incubated with SMase, after which their aggregation, structure, and proteoglycan binding were analyzed. At a molar ratio of L-4F to apoB-100 of 2.5 to 20:1, 4F dose-dependently inhibited SMase-induced LDL aggregation. At a molar ratio of 20:1, SMase-induced aggregation was fully blocked. Binding of 4F to LDL particles inhibited SMase-induced hydrolysis of LDL by 10% and prevented SMase-induced LDL aggregation. In addition, the binding of the SMase-modified LDL particles to human aortic proteoglycans was dose-dependently inhibited by pretreating LDL with 4F. The 4F stabilized apoB-100 conformation and inhibited SMase-induced conformational changes of apoB-100. Molecular dynamic simulations showed that upon binding to protein-free LDL surface, 4F locally alters membrane order and fluidity and induces structural changes to the lipid layer. Collectively, 4F stabilizes LDL particles by preventing the SMase-induced conformational changes in apoB-100 and so blocks SMase-induced LDL aggregation and the resulting increase in LDL retention.

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Publication Forum (2015): 1
Scopus rating (2014): 2.514 1.318
Web of Science (2014): 4.421 5.175 8.5 1.104 0.04284 1.816
Publication Forum (2014): 2
Scopus rating (2013): 2.364 1.364
Publication Forum (2013): 2
Scopus rating (2012): 2.618 1.549
Equipment for obtaining polimeric nanofibres by electrospinning technology: II. The obtaining of polimeric nanofibers

The computerized technologies and equipment for obtaining nanofibers impose high training, a large interdisciplinary substantiation, capacity for data storage, memorizing, easy usage, selectivity, fiability, stability, reduced time for analizing/processing of the technological parameters. That is why the computerized electrospinning equipment and technologies for obtaining nanofibers are possible candidates to carry out these requirements owing to the fact that they present both the proper selectivity/sensibility and the increased processing/determining/intervening speed by using the computerized control. This paper aims to present the operation and application of equipment for obtaining polimeric nanofibers by electrospinning technology. The designing and accomplishing of the suggested electrospinning equipment has been aimed to obtain a modular system which should allow the control of the technological parameters by means of the computer. Thus, the multitude of the parameters which influence the process of electrospinning, can be independently and automatically varied. The obtained nanofibers were studied by scanning electron microscope.

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Authors: Manea, L. R., Cramariuc, B., Popescu, V., Cramariuc, R., Sandu, I., Cramariuc, O.
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Optimization and universality of Brownian search in a basic model of quenched heterogeneous media

The kinetics of a variety of transport-controlled processes can be reduced to the problem of determining the mean time needed to arrive at a given location for the first time, the so-called mean first-passage time (MFPT) problem. The occurrence of occasional large jumps or intermittent patterns combining various types of motion are known to outperform the standard random walk with respect to the MFPT, by reducing oversampling of space. Here we show that a regular but spatially heterogeneous random walk can significantly and universally enhance the search in any spatial dimension. In a generic minimal model we consider a spherically symmetric system comprising two concentric regions with piecewise constant diffusivity. The MFPT is analyzed under the constraint of conserved average dynamics, that is, the spatially averaged diffusivity is kept constant. Our analytical calculations and extensive numerical simulations demonstrate the existence of an optimal heterogeneity minimizing the MFPT to the target. We prove that the MFPT for a random walk is completely dominated by what we term direct trajectories towards the target and reveal a remarkable universality of the spatially heterogeneous search with respect to target size and system dimensionality. In contrast to intermittent strategies, which are most profitable in low spatial dimensions, the spatially inhomogeneous search performs best in higher dimensions. Discussing our results alongside recent experiments on single-particle tracking in living cells, we argue that the observed spatial heterogeneity may be beneficial for cellular signaling processes.
Emergent rogue wave structures and statistics in spontaneous modulation instability

The nonlinear Schrödinger equation (NLSE) is a seminal equation of nonlinear physics describing wave packet evolution in weakly-nonlinear dispersive media. The NLSE is especially important in understanding how high amplitude "rogue waves" emerge from noise through the process of modulation instability (MI) whereby a perturbation on an initial plane wave can evolve into strongly-localised "breather" or "soliton on finite background (SFB)" structures. Although there has been much study of such structures excited under controlled conditions, there remains the open question of how closely the analytic solutions of the NLSE actually model localised structures emerging in noise-seeded MI. We address this question here using numerical simulations to compare the properties of a large ensemble of emergent peaks in noise-seeded MI with the known analytic solutions of the NLSE. Our results show that both elementary breather and higher-order SFB structures are observed in chaotic MI, with the characteristics of the noise-induced peaks clustering closely around analytic NLSE predictions. A significant conclusion of our work is to suggest that the widely-held view that the Peregrine soliton forms a rogue wave prototype must be revisited. Rather, we confirm earlier suggestions that NLSE rogue waves are most appropriately identified as collisions between elementary SFB solutions.

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Authors: Toenger, S., Godin, T., Billet, C., Dias, F., Erkintalo, M., Genty, G., Dudley, J. M.
Ergodicity breaking, ageing, and confinement in generalized diffusion processes with position and time dependent diffusivity

We study generalized anomalous diffusion processes whose diffusion coefficient $D(x, t) \sim D_0|x|^{\alpha}t^{\beta}$ depends on both the position $x$ of the test particle and the process time $t$. This process thus combines the features of scaled Brownian motion and heterogeneous diffusion parent processes. We compute the ensemble and time averaged mean squared displacements of this generalized diffusion process. The scaling exponent of the ensemble averaged mean squared displacement is shown to be the product of the critical exponents of the parent processes, and describes both subdiffusive and superdiffusive systems. We quantify the amplitude fluctuations of the time averaged mean squared displacement as function of the length of the time series and the lag time. In particular, we observe a weak ergodicity breaking of this generalized diffusion process: even in the long time limit the ensemble and time averaged mean squared displacements are strictly disparate. When we start to observe this process some time after its initiation we observe distinct features of ageing. We derive a universal ageing factor for the time averaged mean squared displacement containing all information on the ageing time and the measurement time. External confinement is shown to alter the magnitudes and statistics of the ensemble and time averaged mean squared displacements.

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Simple metal under tensile stress: layer-dependent herringbone reconstruction of thin potassium films on graphite

While understanding the properties of materials under stress is fundamentally important, designing experiments to probe the effects of large tensile stress is difficult. Here tensile stress is created in thin films of potassium (up to 4 atomic layers) by epitaxial growth on a rigid support, graphite. We find that this "simple" metal shows a long-range, periodic "herringbone" reconstruction, observed in 2- and 3- (but not 1- and 4-) layer films by low-temperature scanning tunneling microscopy (STM). Such a pattern has never been observed in a simple metal. Density functional theory (DFT) simulations indicate that the reconstruction consists of self-aligned stripes of enhanced atom density formed to relieve the tensile strain. At the same time marked layer-dependent charging effects lead to substantial variation in the apparent STM layer heights.
Dynamics of rogue wave and soliton emergence in spontaneous modulation instability
Numerical simulations of spontaneous modulation instability show that localized structures in the chaotic instability field are well-described by analytic elementary and higher order soliton on finite background solutions of the nonlinear Schrödinger equation.

Sec14-nodulin proteins and the patterning of phosphoinositide landmarks for developmental control of membrane morphogenesis
Polarized membrane morphogenesis is a fundamental activity of eukaryotic cells. This process is essential for the biology of cells and tissues, and its execution demands exquisite temporal coordination of functionally diverse membrane signaling reactions with high spatial resolution. Moreover, mechanisms must exist to establish and preserve such organization in the face of randomizing forces that would diffuse it. Here we identify the conserved ATSfh1 Sec14-nodulin protein as a novel effector of phosphoinositide signaling in the extreme polarized membrane growth program exhibited by growing Arabidopsis root hairs. The data are consistent with Sec14-nodulin proteins controlling the lateral organization of
phosphatidylinositol 4,5-bisphosphate (PtdIns(4,5)P\(_2\) ) landmarks for polarized membrane morphogenesis in plants. This patterning activity requires both the PtdIns(4,5)P\(_2\) binding and homo-oligomerization activities of the AtSfh1 nodulin domain and is an essential aspect of the polarity signaling program in root hairs. Finally, the data suggest a general principle for how the phosphoinositide signaling landscape is physically bit mapped so that eukaryotic cells are able to convert a membrane surface into a high-definition lipid-signaling screen.

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Publication Forum (2014): 3

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Publication Forum (2013): 3

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Scopus rating (2011): 4.83 1.221

Scopus rating (2010): 5.605 1.286

Scopus rating (2009): 5.779 1.288

Scopus rating (2008): 5.798 1.284

Scopus rating (2007): 6.031 1.335


Scopus rating (2005): 5.965 1.416

Scopus rating (2004): 6.469 1.439

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10.1091/mbc.E14-10-1475
Transbilayer lipid interactions mediate nanoclustering of lipid-anchored proteins

Understanding how functional lipid domains in live cell membranes are generated has posed a challenge. Here, we show that transbilayer interactions are necessary for the generation of cholesterol-dependent nanoclusters of GPI-anchored proteins mediated by membrane-adjacent dynamic actin filaments. We find that long saturated acyl-chains are required for forming GPI-anchor nanoclusters. Simultaneously, at the inner leaflet, long acyl-chain-containing phosphatidylserine (PS) is necessary for transbilayer coupling. All-atom molecular dynamics simulations of asymmetric multicomponent-membrane bilayers in a mixed phase provide evidence that immobilization of long saturated acyl-chain lipids at either leaflet stabilizes cholesterol-dependent transbilayer interactions forming local domains with characteristics similar to a liquid-ordered (lo) phase. This is verified by experiments wherein immobilization of long acyl-chain lipids at one leaflet effects transbilayer interactions of corresponding lipids at the opposite leaflet. This suggests a general mechanism for the generation and stabilization of nanoscale cholesterol-dependent and actin-mediated lipid clusters in live cell membranes.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, National Centre for Biological Sciences (TIFR), Shanmugha Arts Science Technology and Research Academy, Indian Institute of Integrative Medicine (CSIR), Wayne State University, Manipal University Karnataka, Raman Research Institute, Institute for Stem Cell Biology and Regenerative Medicine
Number of pages: 14
Pages: 581-594
Publication date: 23 Apr 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Biochemistry, Genetics and Molecular Biology(all), Medicine(all)

Publication information

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Ratings:
Publication Forum (2017): 3
Publication Forum (2016): 3
Scopus rating (2015): 27.696 5.314
Scopus rating (2014): 28.41 5.687
Web of Science (2014): 32.242 35.532 8.6 5.931 0.57703 19.361
Publication Forum (2014): 3
Scopus rating (2013): 27.895 5.887
Publication Forum (2013): 3
Publication Forum (2012): 3
Scopus rating (2008): 24.783 5.621
Scopus rating (2007): 24.913 5.511
Scopus rating (2006): 23.449 5.496
Scopus rating (2005): 24.633 5.466
Scopus rating (2004): 25.051 5.584
Scopus rating (2003): 27.793 5.482
Ergodicity breaking and particle spreading in noisy heterogeneous diffusion processes
We study noisy heterogeneous diffusion processes with a position dependent diffusivity of the form \( D(x) \sim D_0|\kappa x|^{\alpha_0} \) in the presence of annealed and quenched disorder of the environment, corresponding to an effective variation of the exponent \( \alpha \in [0,\alpha_0] \) in time and space. In the case of annealed disorder, for which effectively \( \alpha(t) = \alpha_0 \), we show how the long time scaling of the ensemble mean squared displacement (MSD) and the amplitude variation of individual realizations of the time averaged MSD are affected by the disorder strength. For the case of quenched disorder, the long time behavior becomes effectively Brownian after a number of jumps between the domains of a stratified medium. In the latter situation, the averages are taken over both an ensemble of particles and different realizations of the disorder. As physical observables, we analyze in detail the ensemble and time averaged MSDs, the ergodicity breaking parameter, and higher order moments of the time averages.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam
Authors: Cherstvy, A. G., Metzler, R.
Publication date: 14 Apr 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

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Volume: 142
Issue number: 14
Article number: 144105
ISSN (Print): 0021-9606
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.073 0.755
Publication Forum (2016): 1
Scopus rating (2015): 0.953 0.767
Web of Science (2015): 2.894 2.95 >10.0 0.786 0.16944 0.873
Publication Forum (2015): 1
Scopus rating (2014): 1.386 0.989
Web of Science (2014): 2.952 3.017 >10.0 0.731 0.18296 0.916
Publication Forum (2014): 3
Scopus rating (2013): 1.532 1.17
Publication Forum (2013): 3
Scopus rating (2012): 1.787 1.118
Publication Forum (2012): 3
Scopus rating (2011): 1.805 1.207
Scopus rating (2010): 1.73 1.052
Scopus rating (2009): 2.003 1.104
Scopus rating (2008): 2.189 1.12
Scopus rating (2007): 2.163 1.108
Scopus rating (2006): 2.176 1.286
Conformational properties of complex polymers: Rosette versus star-like structures

Multiple loop formation in polymer macromolecules is an important feature of the chromatin organization and DNA compactification in the nuclei. We analyse the size and shape characteristics of complex polymer structures, containing in general $f_1$ loops (petals) and $f_2$ linear chains (branches). Within the frames of continuous model of Gaussian macromolecule, we apply the path integration method and obtain the estimates for gyration radius $R_g$ and asphericity $A$ of typical conformation as functions of parameters $f_1$, $f_2$. In particular, our results qualitatively reveal the extent of anisotropy of star-like topologies as compared to the rosette structures of the same total molecular weight.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine
Authors: Blavatska, V., Metzler, R.
Keywords: (conformational properties, path integration, polymers)
Publication date: 7 Apr 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Mathematical Physics, Physics and Astronomy(all), Statistical and Nonlinear Physics, Modelling and Simulation, Statistics and Probability

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Issue number: 13
Article number: 135001
ISSN (Print): 1751-8113
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.879 0.868
Publication Forum (2016): 1
Scopus rating (2015): 0.921 0.963
Web of Science (2015): 1.933 1.591 9.7 0.625 0.04241 0.711
Publication Forum (2015): 1
Scopus rating (2014): 0.92 0.918
Web of Science (2014): 1.583 1.476 9.3 0.615 0.05048 0.714
Publication Forum (2014): 2
Scopus rating (2013): 0.926 1.002
Publication Forum (2013): 2
Scopus rating (2012): 1.016 1.05
Publication Forum (2012): 2
Scopus rating (2011): 0.934 0.946
Scopus rating (2010): 1.056 1.037
N-Glycosylation as determinant of epidermal growth factor receptor conformation in membranes

The epidermal growth factor receptor (EGFR) regulates several critical cellular processes and is an important target for cancer therapy. In lieu of a crystallographic structure of the complete receptor, atomistic molecular dynamics (MD) simulations have recently shown that they can excel in studies of the full-length receptor. Here we present atomistic MD simulations of the monomeric N-glycosylated human EGFR in biomimetic lipid bilayers that are, in parallel, also used for the reconstitution of full-length receptors. This combination enabled us to experimentally validate our simulations, using ligand binding assays and antibodies to monitor the conformational properties of the receptor reconstituted into membranes. We find that N-glycosylation is a critical determinant of EGFR conformation, and specifically the orientation of the EGFR ectodomain relative to the membrane. In the absence of a structure for full-length, posttranslationally modified membrane receptors, our approach offers new means to structurally define and experimentally validate functional properties of cell surface receptors in biomimetic membrane environments.
Word-length entropies and correlations of natural language written texts

We study the frequency distributions and correlations of the word lengths of 10 European languages. Our findings indicate that (a) the word-length distribution of short words quantified by the mean value and the entropy distinguishes the Uralic (Finnish) corpus from the others, (b) the tails at long words, manifested in the high-order moments of the distributions, differentiate the Germanic languages (except for English) from the Romanic languages and Greek and (c) the correlations between nearby word lengths measured by the comparison of the real entropies with those of the shuffled texts are found to be smaller in the case of Germanic and Finnish languages.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Multi-scaled biodata analysis and modelling (MultiBAM), National Technical University of Athens, NCSR, University of Athens, Institute for Language and Speech Processing, Athena R.C.
Authors: Kalimeri, M., Constantoudis, V., Papadimitriou, C., Karamanos, K., Diakonos, F. K., Papageorgiou, H.
Number of pages: 18
Pages: 101-118
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Peer-reviewed: Yes
ASJC Scopus subject areas: Language and Linguistics, Linguistics and Language

Publication information

Journal: Journal of Quantitative Linguistics
Volume: 22
Issue number: 2
ISSN (Print): 0929-6174
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.33 0.918
Publication Forum (2016): 1
Controlled high-fidelity navigation in the charge stability diagram of a double quantum dot

We propose an efficient control protocol for charge transfer in a double quantum dot. We consider numerically a two-dimensional model system, where the quantum dots are subjected to time-dependent electric fields corresponding to experimental gate voltages. Our protocol enables navigation in the charge stability diagram from a state to another through controllable variation of the fields. We show that the well-known adiabatic Landau-Zener transition—when supplemented with a time-dependent field tailored with optimal control theory—can remarkably improve the transition speed. The results also lead to a simple control scheme obtained from the experimental charge stability diagram that requires only a single parameter. Eventually, we can achieve the ultrafast performance of the composite pulse protocol that allows the system to be driven at the quantum speed limit.
Localized surface plasmon resonance in silver nanoparticles: Atomistic first-principles time-dependent density-functional theory calculations

We observe using ab initio methods that localized surface plasmon resonances in icosahedral silver nanoparticles enter the asymptotic region already between diameters of 1 and 2 nm, converging close to the classical quasistatic limit around 3.4 eV. We base the observation on time-dependent density-functional theory simulations of the icosahedral silver clusters Ag55(1.06nm), Ag147(1.60nm), Ag309(2.14nm), and Ag561(2.68 nm). The simulation method combines the adiabatic GLLB-SC exchange-correlation functional with real time propagation in an atomic orbital basis set using the projector-augmented wave method. The method has been implemented for the electron structure code GPAW within the scope of this work. We obtain good agreement with experimental data and modeled results, including photoemission and plasmon resonance. Moreover, we can extrapolate the ab initio results to the classical quasistatically modeled icosahedral clusters.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research group: Electronic Structure Theory, Research area: Computational Physics, Department of Physics, Chalmers University of Technology, COMP Centre of Excellence, Department of Applied Physics, Aalto University, University of Jyväskylä, Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF), Universidad del País Vasco UPV/EHU, CSC-IT Center for Science Ltd.
Authors: Kuisma, M., Sakko, A., Rossi, T. P., Larsen, A. H., Enkovaara, J., Lehtovaara, L., Rantala, T. T.
Keywords: (OPTICAL-PROPERTIES, METAL NANOPARTICLES, AG-CLUSTERS, APPROXIMATION, SIZE, SPECTROSCOPY, ENVIRONMENT, NANOSHELLS, SYSTEMS, SHAPE)
Number of pages: 8
Publication date: 24 Mar 2015
Peer-reviewed: Yes
CO oxidation catalyzed by neutral and anionic Cu20 clusters: Relationship between charge and activity

Reactions of CO and O2 on neutral and anionic Cu20 clusters have been investigated by spin-polarized density functional theory. Three reaction mechanisms of CO oxidation are explored: reactions with atomic oxygen (dissociated O2) as well as reactions with molecular oxygen, including Langmuir-Hinshelwood (LH) and Eley-Rideal (ER) mechanisms. The adsorption energies, reaction pathways, and reaction barriers for CO oxidation are calculated systematically. The anionic Cu20- cluster can adsorb CO and O2 more strongly than the neutral counterpart due to the superatomic shell closing of 20 valence electrons which leaves one electron above the band gap. The activation of O2 molecule upon adsorption is crucial to determine the rate of CO oxidation. The CO oxidation proceeds efficiently on both Cu20 and Cu20- clusters, when O2 is pre-adsorbed dissociatively. The ER mechanism has a lower reaction barrier than the LH mechanism on the neutral Cu20. In general, CO oxidation occurs more readily on the anionic Cu20- (effective reaction barriers 0.1-0.3 eV) than on the neutral Cu20 cluster (0.3-0.5 eV). Moreover, Cu20- exhibits enhanced binding for CO2. From the analysis of the reverse direction of CO oxidation, it is observed that the transition of CO2 to CO + O can occur on the Cu20 cluster, which demonstrates that Cu clusters may serve as good catalyst for CO2 chemistry.
Multiresolution analysis for compactly supported interpolating tensor product wavelets

We construct multidimensional interpolating tensor product multiresolution analyses (MRA’s) of the function spaces $C^0(R^n, K)$, $K = R$ or $K = C$, consisting of real or complex valued functions on $R^n$ vanishing at infinity and the function spaces $C_u(R^n, K)$ consisting of bounded and uniformly continuous functions on $R^n$. We also construct an interpolating dual MRA for both of these spaces. The theory of the tensor products of Banach spaces is used. We generalize the Besov space norm equivalence from the one-dimensional case to our $n$-dimensional construction.

General information
Resveratrol interferes with the aggregation of membrane-bound human-IAPP: A molecular dynamics study

Amyloid aggregation of islet amyloid polypeptide (IAPP) in pancreatic tissues is a typical feature of type 2 diabetes mellitus. Resveratrol, a natural product extensively studied for its wide range of biological effects, has been shown to inhibit IAPP aggregation. However, the mechanism by which resveratrol inhibits IAPP aggregation is still far from complete elucidation. Now, an increasing knowledge of the mechanism of amyloid toxicity shifts the target of research towards the development of compounds which can prevent amyloid-mediated membrane damage rather than merely inhibit fiber formation. In this study we used all atom molecular dynamics to investigate the interaction of resveratrol with full-length human IAPP in a negatively charged membrane environment. Our results show that the presence of resveratrol induces the formation of secondary structures (sheets and helices) by inserting in a hydrophobic pocket between the interaction surface of two IAPP molecules in aqueous solution. On the other hand, resveratrol significantly perturbs the interaction of IAPP with negatively charged membranes by anchoring specific hydrophobic regions (23FGA25 and 32VGS34) of the peptide and forming a stable 1:2 IAPP:resveratrol complex at the water/membrane interphase.
Suppression of strong-field ionization by optimal pulse shaping: Application to hydrogen and the hydrogen molecular ion

We investigate the ability of quantum optimal control theory to shape pulses suppressing strong-field ionization of a hydrogen atom and a H-$2^+(\ast)$ molecule. We show that considerable suppression of the ionization yield can be achieved for both H and H-$2^+(\ast)$ with optimal pulse shaping for a fixed fluence and pulse length. The mechanisms responsible for ionization suppression and the shape of the optimized pulse are different for infrared and ultraviolet laser fields. In the low-frequency regime the optimized pulse reduces the ionization yield by suppressing the highest peaks of the laser field. For the higher laser frequencies considered the ionization yield of H can be decreased by exciting low-lying resonances.

General information
Polymer looping is controlled by macromolecular crowding, spatial confinement, and chain stiffness

We study by extensive computer simulations the looping characteristics of linear polymers with varying persistence length inside a spherical cavity in the presence of macromolecular crowding. For stiff chains, the looping probability and looping time reveal wildly oscillating patterns as functions of the chain length. The effects of crowding differ dramatically for flexible versus stiff polymers. While for flexible chains the looping kinetics is slowed down by the crowders, for stiffer chains the kinetics turns out to be either decreased or facilitated, depending on the polymer length. For severe confinement, the looping kinetics may become strongly facilitated by crowding. Our findings are of broad impact for DNA looping in the
Resolving unoccupied electronic states with laser ARPES in bismuth-based cuprate superconductors

Angle-resolved photoemission spectroscopy (ARPES) is typically used to study only the occupied electronic band structure of a material. Here we use laser-based ARPES to observe a feature in bismuth-based superconductors that, in contrast, is related to the unoccupied states. Specifically, we observe a dispersive suppression of intensity cutting across the valence band, which, when compared with relativistic one-step calculations, can be traced to two final-state gaps in the bands 6 eV above the Fermi level. This finding opens up possibilities to bring the ultrahigh momentum resolution of existing laser-ARPES instruments to the unoccupied electron states. For cases where the final-state gap is not the object of study, we find that its effects can be made to vanish under certain experimental conditions.
Real-space Wigner-Seitz Cells Imaging of Potassium on Graphite via Elastic Atomic Manipulation

Atomic manipulation in the scanning tunnelling microscopy, conventionally a tool to build nanostructures one atom at a time, is here employed to enable the atomic-scale imaging of a model low-dimensional system. Specifically, we use low-temperature STM to investigate an ultra thin film (4 atomic layers) of potassium created by epitaxial growth on a graphite substrate. The STM images display an unexpected honeycomb feature, which corresponds to a real-space visualization of the Wigner-Seitz cells of the close-packed surface K atoms. Density functional simulations indicate that this behaviour arises from the elastic, tip-induced vertical manipulation of potassium atoms during imaging, i.e. elastic atomic manipulation, and reflects the ultrasoft properties of the surface under strain. The method may be generally applicable to other soft e.g. molecular or biomolecular systems.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research group: Materials and Molecular Modeling, Computational Science X (CompX), Univ Birmingham, University of Birmingham, Sch Phys & Astron, Nanoscale Phys Res Lab, Shaanxi Normal Univ, Shaanxi Normal University, Sch Phys & Informat Technol, Univ Jyvaskyla, University of Jyvaskyla, Dept Phys, Nanosci Ctr, Aalto Univ, Aalto University, Sch Sci, COMP Ctr Excellence, Dept Appl Phys
Authors: Yin, F., Koskinen, P., Kulju, S., Akola, J., Palmer, R. E.
Semantic Labeling of Places based on Phone Usage Features using Supervised Learning

Nowadays mobile applications demand higher context awareness. The applications aim to understand the user’s context (e.g., home or at work) and provide services tailored to the users. The algorithms responsible for inferring the user’s context are the so-called context inference algorithms, the place detection being a particular case. Our hypothesis is that people use mobile phones differently when they are located in different places (e.g. longer calls at home than at work). Therefore, the usage of the mobile phones could be an indicator of the users’ current context. The objective of the work is to develop a system that can estimate the user's place label (home, work, etc.), based on phone usage. As training and validation set, we use a database containing phone usage information of 200 users over several months including phone call and SMS logs, multimedia usage, accelerometer, GPS, network information and system information. The data was split into visits, i.e., periods of uninterrupted time that the user has been in a certain place (Home, Work, Leisure, etc.). The data include information about the phone usage during the visits, and the semantic label of the place visited (Home, Work, etc.). We consider two approaches to represent this data: the first approach (so-called visits approach) saves each visit separately; the second approach (so-called places approach) combines all visits of one user to a certain place and creates place-specific information. For place detection, we used five popular classification methods, Naive Bayes, Decision Tree, Bagged Tree, Neural Network and K-Nearest Neighbors, in both representation approaches. We evaluated their classification rates and found that: 1) Bagged Tree outperforms the other methods; 2) the places data-representation gives better results than the visits data-representation.
Integrated in vitro-in silico screening strategy for the discovery of antibacterial compounds

Multidrug-resistant bacterial infections are an increasing source of healthcare problems, and the research for new antibiotics is currently unable to respond to this challenge. In this work, we present a screening strategy that integrates cell-based high-throughput screening (HTS) with in silico analogue search for antimicrobial small-molecule drug discovery. We performed an HTS on a diverse chemical library by using an assay based on a bioluminescent Escherichia coli K-12 (pTetLux1) strain. The HTS yielded eight hit compounds with >50% inhibition. These hits were then used for structural similarity-based virtual screening, and of the 29 analogues selected for in vitro testing, four compounds displayed potential activity in the pTetLux1 assay. The 11 most active compounds from combined HTS and analogue search were further assessed for antimicrobial activity against clinically important strains of E. coli and Staphylococcus aureus and for in vitro cytotoxicity against human cells. Three of the compounds displayed antibacterial activity and low human cell cytotoxicity. Additionally, two compounds of the set fully inhibited S. aureus growth after 24 h, but also exhibited human cell cytotoxicity in vitro.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Tampere University of Technology, Urban circular bioeconomy (UrCirBio), Centre for Drug Research, Division of Pharmaceutical Biosciences, Helsinki University, Division of Pharmaceutical Chemistry and Technology
Authors: Nybond, S., Ghemtio, L., Nawrot, D. A., Karp, M., Xhaard, H., Tammela, P.
Number of pages: 9
Pages: 25-33
Publication date: 1 Feb 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Drug Discovery, Molecular Medicine

Publication information
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Volume: 13
Issue number: 1
ISSN (Print): 1540-658X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.832 0.605
Publication Forum (2016): 1
Scopus rating (2015): 0.839 0.65
The looping of polymers such as DNA is a fundamental process in the molecular biology of living cells, whose interior is characterised by a high degree of molecular crowding. We here investigate in detail the looping dynamics of flexible polymer chains in the presence of different degrees of crowding. From the analysis of the looping-unlooping rates and the looping probabilities of the chain ends we show that the presence of small crowders typically slows down the chain dynamics but larger crowders may in fact facilitate the looping. We rationalise these non-trivial and often counterintuitive effects of the crowder size on the looping kinetics in terms of an effective solution viscosity and standard excluded volume. It is shown that for small crowders the effect of an increased viscosity dominates, while for big crowders we argue that confinement effects (caging) prevail. The tradeoff between both trends can thus result in the impediment or facilitation of polymer looping, depending on the crowder size. We also examine how the crowding volume fraction, chain length, and the attraction strength of the contact groups of the polymer chain affect the looping kinetics and hairpin formation dynamics. Our results are relevant for DNA looping in the absence and presence of protein mediation, DNA hairpin formation, RNA folding, and the folding of polypeptide chains under biologically relevant high-crowding conditions.
Non-universal tracer diffusion in crowded media of non-inert obstacles

We study the diffusion of a tracer particle, which moves in continuum space between a lattice of excluded volume, immobile non-inert obstacles. In particular, we analyse how the strength of the tracer-obstacle interactions and the volume occupancy of the crowders alter the diffusive motion of the tracer. From the details of partitioning of the tracer diffusion modes between trapping states when bound to obstacles and bulk diffusion, we examine the degree of localisation of the tracer in the lattice of crowders. We study the properties of the tracer diffusion in terms of the ensemble and time averaged mean squared displacements, the trapping time distributions, the amplitude variation of the time averaged mean squared displacements, and the non-Gaussianity parameter of the diffusing tracer. We conclude that tracer-obstacle adsorption and binding triggers a transient anomalous diffusion. From a very narrow spread of recorded individual time averaged trajectories we exclude continuous type random walk processes as the underlying physical model of the tracer diffusion in our system. For moderate tracer-crowder attraction the motion is found to be fully ergodic, while at stronger attraction strength a transient disparity between ensemble and time averaged mean squared displacements occurs. We also put our results into perspective with findings from experimental single-particle tracking and simulations of the diffusion of tagged tracers in dense crowded suspensions. Our results have implications for the diffusion, transport, and spreading of chemical components in highly crowded environments inside living cells and other structured liquids.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam
Authors: Ghosh, S. K., Cherstvy, A. G., Metzler, R.
Number of pages: 12
Pages: 1847-1858
Publication date: 21 Jan 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 17
Issue number: 3
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Testing the near field/far field model performance for prediction of particulate matter emissions in a paint factory

A Near Field/Far Field (NF/FF) model is a well-accepted tool for precautionary exposure assessment but its capability to estimate particulate matter (PM) concentrations is not well studied. The main concern is related to emission source characterization which is not as well defined for PM emitters compared to e.g. for solvents. One way to characterize PM emission source strength is by using the material dustiness index which is scaled to correspond to industrial use by using modifying factors, such as handling energy factors. In this study we investigate how well the NF/FF model predicts PM concentration levels in a paint factory. PM concentration levels were measured during big bag and small bag powder pouring. Rotating drum dustiness indices were determined for the specific powders used and applied in the NF/FF model to predict mass concentrations. Modeled process specific concentration levels were adjusted to be similar to the measured concentration levels by adjusting the handling energy factor. The handling energy factors were found to vary considerably depending on the material and process even though they have the same values as modifying factors in the exposure models. This suggests that the PM source characteristics and process-specific handling energies should be studied in more detail to improve the model-based exposure assessment.

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Danmarks Tekniske Universitet, DTU Informatik, Denmark Technical University DTU, National Research Centre for the Working Environment, Department of Micro and Nanotechnology
Number of pages: 12
Pages: 62-73
Publication date: 1 Jan 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Environmental Chemistry, Public Health, Environmental and Occupational Health, Management, Monitoring, Policy and Law, Medicine(all)
Weak ergodicity breaking and ageing in anomalous diffusion

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research area: Computational Physics
Authors: Metzler, R.
Number of pages: 16
Pages: 1560007
Publication date: 1 Jan 2015
Peer-reviewed: Yes

Publication Information
Journal: Journal of Physics: Conference Series
Volume: 36
ISSN (Print): 1742-6588
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.24 0.383
Scopus rating (2015): 0.24 0.373
Scopus rating (2014): 0.253 0.344
Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory

A key component in calculations of exchange and correlation energies is the Coulomb operator, which requires the evaluation of two-electron integrals. For localized basis sets, these four-center integrals are most efficiently evaluated with the resolution of identity (RI) technique, which expands basis-function products in an auxiliary basis. In this work we show the practical applicability of a localized RI-variant (‘RI-LVL’), which expands products of basis functions only in the subset of those auxiliary basis functions which are located at the same atoms as the basis functions. We demonstrate the accuracy of RI-LVL for Hartree–Fock calculations, for the PBE0 hybrid density functional, as well as for RPA and MP2 perturbation theory. Molecular test sets used include the S22 set of weakly interacting molecules, the G3 test set, as well as the G2–1 and BH76 test sets, and heavy elements including titanium dioxide, copper and gold clusters. Our RI-LVL implementation paves the way for linear-scaling RI-based hybrid functional calculations for large systems and for all-electron many-body perturbation theory with significantly reduced computational and memory cost.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research area: Computational Physics, Computational Science X (CompX)
Authors: Ihrig, A. C., Wieferink, J., Zhang, I. Y., Ropo, M., Ren, X., Rinke, P., Scheffler, M., Blum, V.
Number of pages: 20
Publication date: 2015
Peer-reviewed: Yes

Publication information

Journal: New Journal of Physics
Volume: 17
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Article number: 093020
ISSN (Print): 1367-2630
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.788 1.031
Publication Forum (2016): 2
Scopus rating (2015): 1.938 1.047
Web of Science (2015): 3.57 3.501 4.7 1.118 0.10691 1.706
Publication Forum (2015): 2
Scopus rating (2014): 2.806 1.307
Web of Science (2014): 3.558 3.664 4.4 0.861 0.12987 1.982
Publication Forum (2014): 2
Scopus rating (2013): 2.871 1.372
Publication Forum (2013): 2
Scopus rating (2012): 3.352 1.533
Publication Forum (2012): 2
Scopus rating (2011): 3.47 1.634
Scopus rating (2010): 3.395 1.421
A model for anisotropic magnetostriction

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Department of Mechanical Engineering and Industrial Systems, Research area: Applied Mechanics, Lund University, Aalto University
Authors: Belahcen, A., Kouhia, R., Rasilo, P., Ristinmaa, M.
Number of pages: 3
Pages: 201-203
Publication date: 2015

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Publisher: Rakenteiden Mekaniikan Seura ry
ISBN (Print): 978-952-93-5608-9

Bibliographical note
EXT="Rasilo, Paavo"
Research output: Scientific › Conference contribution

A new method to calculate natural convection heat transfer from a non-isothermal fin array

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Mechanical Engineering and Industrial Systems, Research area: Applied Mechanics, Research group: Lämpö- ja virtaustekniikka
Authors: Lampio, K., Karvinen, R.
Publication date: 2015

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Title of host publication: Proceedings of the 7th Baltic Heat Transfer Conference, August 24-26 2015, Tallinn Estonia
Place of publication: Tallinn
Publisher: Tallinn University of Technology
Editors: Neshumayev, D., Sunden, B.
ISBN (Print): 978-9949-23-617-0

Publication series
Name: Baltic Heat Transfer Conference BHTC
Publisher: Tallinn University of Technology
Computational modelling of high-cycle fatigue using a continuum based model
In this paper a computational implementation of continuum based transversally isotropic fatigue model is described. The key idea of the continuum based HCF-model is the moving endurance surface where the movement is described by a back stress type tensor, the evolution of which is described by a rate type equation. Furthermore, damage accumulation is also governed with a rate type evolution equation. The model is implemented in the Abaqus FE-program using the user material subroutine. Two strategies to perform a fatigue analysis are compared in a standard cycling loading case. The first analysis reflects the procedure used in a standard fatigue computation. In the second analysis type the effect of evolving damage fields on fatigue life is investigated.

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Department of Mechanical Engineering and Industrial Systems, Research area: Applied Mechanics
Authors: Holopainen, S., Kouhia, R., Könnö, J., Saksala, T.
Number of pages: 4
Pages: 71-74
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the NSCM28 : 28th Nordic Seminar on Computational Mechanics, October 22 – 23, 2015, Tallinn, Estonia
ISBN (Print): 978-9949-430-95-6
Electronic versions:
Holopainen_etal_NSCM28
Links:
http://urn.fi/URN:NBN:fi:tty-201610194608

Bibliographical note
oa 2015 Holopainen et al tarkistettu 19.10.2016 /KK
Research output: Scientific › Conference contribution

Damage-viscoplastic model based on the Hoek-Brown criterion for numerical modeling of rock fracture
This article presents a phenomenological damage-viscoplastic model based on the empirical Hoek-Brown criterion for numerical modeling of rock fracture. The viscoplastic part of the model is formulated in the spirit of the consistency model by Wang (1997). Isotropic damage model with separate damage variables in tension and compression is employed to describe the stiffness and strength degradation. The model is implemented with the FE method using the constant strain triangle elements. The equations of motion are solved with the explicit time marching scheme. In the numerical examples, after demonstrating the model response at the material point level, confined compression and uniaxial tension tests on rock are simulated as quasi-static problems. Moreover, the dynamic three-point bending of a notched semicircular disc test is simulated in order to demonstrate the model predictions under dynamic loading conditions.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Mechanical Engineering and Industrial Systems, Research area: Applied Mechanics, Research group: Teknillinen mekaniikka ja lujuusoppi
Authors: Saksala, T.
Number of pages: 16
Pages: 99-114
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Rakenteiden mekaniikka
Volume: 48
Issue number: 2
ISSN (Print): 0783-6104
Ratings:
Publication Forum (2017): 1
Data Rate Performance of Droplet Microfluidic Communication System

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Authors: Wirdatmadja, S., Moltchanov, D., Bolcos, P., Väliaho, J., Kreutzer, J., Kallio, P., Koucheryavy, Y.
Pages: 5:1-5:6
Publication date: 2015

Host publication information
Title of host publication: NANOCON' 15, Proceedings of the Second Annual International Conference on Nanoscale Computing and Communication
Place of publication: New York, NY, USA
Publisher: ACM
ISBN (Print): 978-1-4503-3674-1
DOIs: 10.1145/2800795.2800808

Bibliographical note
ORG=elt,0.5
ORG=ase,0.5
Source: Bibtex
Source-ID: urn:04611a69237f0b418864f7c31d126c53
Research output: Scientific - peer-review › Conference contribution

Dynamics of Epithelial Tight Junction as Molecular and Electric Barrier - A Computational Approach

General information
State: Published
Organisations: Department of Electronics and Communications Engineering, Research group: Computational Biophysics and Imaging Group
Authors: Tervonen, A., Nymark, S., Leon, D. G., Onnela, N. M., Hyttinen, J.
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Investigative Ophthalmology and Visual Science
Volume: 56
Issue number: 7
ISSN (Print): 0146-0404
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.836 1.283
Publication Forum (2016): 2
Scopus rating (2015): 2.04 1.408
Web of Science (2015): 3.427 3.732 7.7 0.576 0.08427 1.107
Experimental determination and computational interpretation of biophysical properties of lipid bilayers enriched by cholesteryl hemisuccinate

Cholesteryl hemisuccinate (CHS) is one of the cholesterol-mimicking detergents not observed in nature. It is, however, widely used in protein crystallography, in biochemical studies of proteins, and in pharmacology. Here, we performed an extensive experimental and theoretical study on the behavior of CHS in lipid membranes rich in unsaturated phospholipids. We found that the deprotonated form of CHS (that is the predominant form under physiological conditions) does not mimic cholesterol very well. The protonated form of CHS does better in this regard, but also its ability to mimic the physical effects of cholesterol on lipid membranes is limited. Overall, although ordering and condensing effects characteristic to cholesterol are present in systems containing any form of CHS, their strength is appreciably weaker compared to cholesterol. Based on the considerable amount of experimental and atomistic simulation data, we conclude that these differences originate from the fact that the ester group of CHS does not anchor it in an optimal position at the water-membrane interface. The implications of these findings for considerations of protein-cholesterol interactions are briefly discussed.

General information

State: Published

Ministry of Education publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, University of Southern Denmark

Authors: Kulig, W., Jurkiewicz, P., Olzyńska, A., Tynkkynen, J., Javanainen, M., Manna, M., Rog, T., Hof, M., Vattulainen, I., Jungwirth, P.

Keywords: (Cholesterol-mimicking detergents, DPH, Dynamic light scattering, Laurdan, Molecular dynamics simulations, Time-dependent fluorescence shift)

Number of pages: 11

Pages: 422-432

Publication date: 2015

Peer-reviewed: Yes

Early online date: 25 Oct 2014

ASJC Scopus subject areas: Biochemistry, Cell Biology, Biophysics, Medicine(all)

Publication information

Journal: Biochimica et Biophysica Acta: Biomembranes

Volume: 1848

Issue number: 2

ISSN (Print): 0005-2736
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.511 1.101
Publication Forum (2016): 1
Scopus rating (2015): 1.782 1.142
Web of Science (2015): 3.687 3.589 7.3 0.907 0.02731 1.163
Publication Forum (2015): 1
Scopus rating (2014): 1.869 1.09
Web of Science (2014): 3.836 3.881 7.0 1.006 0.02991 1.257
Publication Forum (2014): 2
Scopus rating (2013): 1.592 0.975
Publication Forum (2013): 2
Scopus rating (2012): 1.833 1.156
Publication Forum (2012): 2
Scopus rating (2011): 1.644 1.227
Scopus rating (2009): 2.152 1.298
Scopus rating (2008): 2.035 1.123
Scopus rating (2007): 2.021 1.158
Scopus rating (2005): 2.037 1.231
Scopus rating (2004): 1.5 1.147
Scopus rating (2003): 1.401 1.115
Scopus rating (2002): 1.594 1.228
Scopus rating (2001): 1.509 1.053
Scopus rating (2000): 1.089 0.907
Scopus rating (1999): 0.95 0.841
Original language: English
DOIs:
10.1016/j.bbamem.2014.10.032
Links:
http://www.scopus.com/inward/record.url?scp=84912099904&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note
AUX=fys,"Tynkkynen, Joona"
Source: Scopus
Source-ID: 84912099904
Research output: Scientific - peer-review › Article

Exploration of different boundary conditions in the sideways falling situation in hip fracture finite element modelling

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Department of Mechanical Engineering and Industrial Systems, Research area: Applied Mechanics, Department of Electronics and Communications Engineering, Research group: Computational Biophysics and Imaging Group, BioMediTech, UKK Institute for Health Promotion Research
Authors: Abe, S., Ylinen, A., Narra Girish, N., Nikander, R., Hyttilä, J., Kouhia, R., Sievänen, H.
Number of pages: 6
Pages: 130-135
Publication date: 2015

Host publication information
Title of host publication: Proceeding of the XII Finnish Mechanics Days
Publisher: Rakenteiden Mekaniikan Seura ry
ISBN (Print): 978-952-93-5608-9
Links:
Facilitation of polymer looping and giant polymer diffusivity in crowded solutions of active particles
We study the dynamics of polymer chains in a bath of self-propelled particles (SPP) by extensive Langevin dynamics simulations in a two-dimensional model system. Specifically, we analyse the polymer looping properties versus the SPP activity and investigate how the presence of the active particles alters the chain conformational statistics. We find that SPPs tend to extend flexible polymer chains, while they rather compactify stiffer semiflexible polymers, in agreement with previous results. Here we show that higher activities of SPPs yield a higher effective temperature of the bath and thus facilitate the looping kinetics of a passive polymer chain. We explicitly compute the looping probability and looping time in a wide range of the model parameters. We also analyse the motion of a monomeric tracer particle and the polymer’s centre of mass in the presence of the active particles in terms of the time averaged mean squared displacement, revealing a giant diffusivity enhancement for the polymer chain via SPP pooling. Our results are applicable to rationalising the dimensions and looping kinetics of biopolymers at constantly fluctuating and often actively driven conditions inside biological cells or in suspensions of active colloidal particles or bacteria cells.
Geometry controlled anomalous diffusion in random fractal geometries: Looking beyond the infinite cluster

We investigate the ergodic properties of a random walker performing (anomalous) diffusion on a random fractal geometry. Extensive Monte Carlo simulations of the motion of tracer particles on an ensemble of realisations of percolation clusters are performed for a wide range of percolation densities. Single trajectories of the tracer motion are analysed to quantify the time averaged mean squared displacement (MSD) and to compare this with the ensemble averaged MSD of the particle motion. Other complementary physical observables associated with ergodicity are studied, as well. It turns out that the time averaged MSD of individual realisations exhibits non-vanishing fluctuations even in the limit of very long observation times as the percolation density approaches the critical value. This apparent non-ergodic behaviour concurs with the ergodic behaviour on the ensemble averaged level. We demonstrate how the non-vanishing fluctuations in single particle trajectories are analytically expressed in terms of the fractal dimension and the cluster size distribution of the random geometry, thus being of purely geometrical origin. Moreover, we reveal that the convergence scaling law to ergodicity, which is known to be inversely proportional to the observation time \( T \) for ergodic diffusion processes, follows a power-law \( \sim T^{-h} \) with \( h < 1 \) due to the fractal structure of the accessible space. These results provide useful measures for differentiating the subdiffusion on random fractals from an otherwise closely related process, namely, fractional Brownian motion. Implications of our results on the analysis of single particle tracking experiments are provided.
How endoglucanase enzymes act on cellulose nanofibrils: role of amorphous regions revealed by atomistic simulations

Transformation of cellulose into monosaccharides can be achieved in a chemical process performed by a special group of enzymes known as cellulases. We have used atomistic molecular dynamics simulations to study endoglucanase II (Cel5A) that is one of the proteins in this group. Based on the atomistic simulation results, we discuss how the Cel5A enzyme interacts with cellulose fibrils comprised of both crystalline and amorphous regions. We show that the enzyme’s carbohydrate-binding domain prefers to interact with crystalline regions of cellulose, while the catalytic domain has a high affinity to the amorphous regions of fibrils. In particular, through electrostatic interactions the catalytic domain attracts loose glucose chains to its catalytic cleft. The atomistic details of the enzyme–cellulose interaction are presented and the implications for practical applications are briefly discussed.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), Lappeenranta University of Technology, University of Jyväskylä, Stora Enso, Department of Physics and Nanoscience Center
Authors: Orłowski, A., Rög, T., Paavilainen, S., Manna, M., Heiskanen, I., Backfolk, K., Timonen, J., Vattulainen, I.
Keywords: (Cellulose, Enzyme, Molecular dynamics simulation)
Number of pages: 15
Pages: 2911-2925
Publication date: 2015
Peer-reviewed: Yes
Early online date: 17 Jul 2015
ASJC Scopus subject areas: Polymers and Plastics

Publication information
Journal: Cellulose
Volume: 22
Issue number: 5
ISSN (Print): 0969-0239
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.126 1.144
Publication Forum (2016): 2
Web of Science (2015): 3.195 3.741 4.6 0.521 0.01196 0.722
Publication Forum (2015): 2
Scopus rating (2014): 1.071 1.334
Web of Science (2014): 3.573 4.285 4.6 0.655 0.00994 0.773
Publication Forum (2014): 2
Scopus rating (2013): 1.127 1.48
Publication Forum (2013): 2
Scopus rating (2012): 1.179 1.71
Publication Forum (2012): 2
Scopus rating (2011): 1.354 1.795
Insights into the behavioral difference of water in the presence of GM1

Studies on the structure and dynamics of interfacial water, emphasizing on the properties of water near the surface of biomolecules, are well reported, but there is a lack of evidence on the behavior of water near a comparatively rough surface containing molecules with a bulky head group like GM1. In this report we comparatively analyze the structure and dynamics of water as a function of distance from the lipid head group in GM1 containing lipid bilayers, with the lipid bilayers where GM1 is not present. This approach effectively demonstrates the behavioral difference and hence delayed convergence from bound water to bulk water in the presence of GM1 compared to a relatively smooth surface.
Memory effect in crystallization of amorphous Ge2Sb2Te5

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Physics, Research area: Computational Physics, Research group: Materials and Molecular Modeling, Forschungszentrum Jülich (FZJ)
Authors: Akola, J., Kalikka, J., Jones, R. O.
Number of pages: 6
Pages: 46-51
Publication date: 2015

Host publication information
Title of host publication: EPJ3O2015 Proceedings
Research output: Professional › Conference contribution

Numerical modelling of rock fracture with the embedded discontinuity approach incorporating heterogeneity

In this paper, the embedded discontinuity approach is applied to finite element modeling of rock fracture. A rate-dependent constitutive model based on the embedded displacement discontinuity theory is developed to describe the mode I, mode II and mixed mode fracture of rock in tension and compression. The bulk material is described as linear elastic until reaching the elastic limit. Beyond this limit, a rate-dependent exponential softening law governs the evolution of the embedded displacement jump. The present approach incorporates the rock heterogeneity by random description of the mineral texture of rock. Moreover, the inherent initial microcrack populations of natural rocks are accounted for as randomly oriented embedded discontinuities. Numerical examples demonstrate the model behavior in uniaxial compression and tension. The effect of loading rate and confining pressure is tested as well in 2D numerical simulations. These simulations show that the model captures the main features of rock in confined compression and uniaxial tension. The developed method has the computational efficiency of continuum plasticity models. However, it has an important advantage of accounting for the orientation of introduced microcracks.

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Mechanical Engineering and Industrial Systems, Research area: Applied Mechanics
Authors: Saksala, T.
Number of pages: 11
Publication date: 2015

Host publication information
Publisher: International Society for Rock Mechanics ISRM
Planning-based semantic web service composition in factory automation

The Service Oriented Architecture (SOA) paradigm enables production systems to be composed of web services. In an SOA-based production system, the individual production devices provide web service interfaces that encapsulate the behavior of the devices and abstract the implementation details. Such a service-oriented approach makes it possible to apply web service orchestration technologies in the development of production workflow descriptions. While manual formulation of production workflows tends to require considerable effort from domain experts, semantic web service descriptions enable computer algorithms to automatically generate the appropriate web service orchestrations. Such algorithms realize AI planning and employ semantic web service descriptions in determining the workflows required to achieve the production goals desired. In addition, the algorithms can automatically adapt the workflows to unexpected changes in the goals pursued and the production devices available.
The Prototype Phase Change Material Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}: Amorphous structure and crystallization

The widespread use of phase change materials in storage media is based on the extremely rapid and reversible switching between the amorphous and crystalline phases of some families of semiconducting alloys. Detailed information about the structure of the amorphous phase and the mechanism of crystallization are essential for the development of new storage media, and we study both aspects here using density functional/molecular dynamics simulations of Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}, the prototype phase change material of the Ge/Sb/Te semiconductor family.

Toward Atomistic Resolution Structure of Phosphatidylcholine Headgroup and Glycerol Backbone at Different Ambient Conditions

Phospholipids are essential building blocks of biological membranes. Despite a vast amount of very accurate experimental data, the atomistic resolution structures sampled by the glycerol backbone and choline headgroup in phosphatidylcholine bilayers are not known. Atomistic resolution molecular dynamics simulations have the potential to resolve the structures, and to give an arresting intuitive interpretation of the experimental data, but only if the simulations reproduce the data within experimental accuracy. In the present work, we simulated phosphatidylcholine (PC) lipid bilayers with 13 different atomistic models, and compared simulations with NMR experiments in terms of the highly structurally sensitive C-H bond order parameters. Focusing on the glycerol backbone and choline headgroups, we showed that the order parameter comparison can be used to judge the atomistic resolution structural accuracy of the models. Accurate models, in turn, allow molecular dynamics simulations to be used as an interpretative tool that translates these NMR data into a dynamic three-dimensional representation of biomolecules in biologically relevant conditions. In addition to lipid bilayers in fully hydrated conditions, we reviewed previous experimental data for dehydrated bilayers and cholesterol-containing bilayers, and interpreted them with simulations. Although none of the existing models reached experimental accuracy, by critically comparing them we were able to distill relevant chemical information: (1) increase of choline order parameters indicates the P-N vector tilting more parallel to the membrane, and (2) cholesterol induces only minor changes to the PC (glycerol backbone) structure. This work has been done as a fully open collaboration, using nmrlipids.blogspot.fi as a communication platform; all the scientific contributions were made publicly on this blog. During the open research process,
The repository holding our simulation trajectories and files (https://zenodo.org/collection/user-nmrlipids) has become the most extensive publicly available collection of molecular dynamics simulation trajectories of lipid bilayers.
Unsteady turbulent boundary layers in swimming rainbow trout

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Applied Mechanics, Department of Mechanical Engineering and Industrial Systems
Authors: Yanase, K., Saarenrinne, P.
Pages: 1373-1385
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Journal of Experimental Biology
Volume: 218
Issue number: 9
ISSN (Print): 0022-0949
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.722 1.279
Publication Forum (2016): 2
Scopus rating (2015): 1.812 1.222
Web of Science (2015): 2.914 3.207 >10.0 1.023 0.04003 1.107
Publication Forum (2015): 2
Scopus rating (2014): 1.722 1.331
Web of Science (2014): 2.897 3.345 9.8 0.913 0.04016 1.085
Publication Forum (2014): 2
Scopus rating (2013): 1.719 1.323
Publication Forum (2013): 2
Scopus rating (2012): 1.612 1.395
Publication Forum (2012): 2
Scopus rating (2011): 1.534 1.315
Scopus rating (2010): 1.474 1.341
Scopus rating (2009): 1.764 1.365
How mono-valent cations bend peptide turns and a first-principles database of amino acids and dipeptides

In this contribution we detail our efforts to investigate the structural effects of cations binding to peptides and amino acids. We perform first-principles studies employing long-range dispersion-corrected approximate density-functional theory and compare to gas-phase experiments.

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Physics, Research area: Computational Physics, Computational Science X (CompX), Fritz Haber Institute of the Max Planck Society, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Duke University
Authors: Baldauf, C., Ropo, M., Blum, V., Scheffler, M.
Keywords: (benchmarks, conformation database, density-functional theory, Peptide conformation, theoretical vibrational spectroscopy)
Number of pages: 2
Pages: 119-120
Publication date: 6 Oct 2014

Host publication information
Title of host publication: International Conference of Computational Methods in Sciences and Engineering 2014 (ICCMSE 2014)
Volume: 1618
Publisher: American Institute of Physics Inc.
Editors: Simos, T. E., Kalogiratou, Z., Monovasilis, T.
ISBN (Print): 9780735412552
ASJC Scopus subject areas: Physics and Astronomy(all)

Publication series
Name: AIP Conference Proceedings
Volume: 1618
ISSN (Print): 0094-243X
DOIs:
10.1063/1.4897692
Source: Scopus
Source-ID: 84947544071
Research output: Scientific - peer-review › Conference contribution

A case study of share of ICT infrastructure in energy consumption of discrete manufacturing facility

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Mechanical Engineering and Industrial Systems, Research group: Factory automation systems technology
Authors: Sohail, M., Florea, A., Martinez Lastra, J. L.
Number of pages: 6
Pages: 1-6
A Continuum damage model based on Ottosen's four parameter failure criterion for concrete

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Mechanical Engineering and Industrial Systems
Authors: Tahaei Yaghoubi, S., Kouhia, R., Hartikainen, J., Kolari, K.
Number of pages: 17
Pages: 50-66
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Rakenteiden mekaniikka
Volume: 47
Issue number: 2
ISSN (Print): 0783-6104
Ratings:
Publication Forum (2017): 1
Publication Forum (2016): 1
Publication Forum (2015): 1
Publication Forum (2014): 1
Publication Forum (2013): 1
Publication Forum (2012): 1
Original language: English
Links:

Bibliographical note
Contribution: organisation=mei,FACT1=1<br>Portfolio EDEND: 2014-12-15<br>Publisher name: Rakenteiden Mekaniikan Seura
Source: researchoutputwizard
Source-ID: 1591
Research output: Scientific - peer-review › Article

A Continuum damage model for quasi-brittle materials

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Mechanical Engineering and Industrial Systems
Authors: Yaghoubi, S. T., Kouhia, R., Hartikainen, J., Kolari, K.
Number of pages: 4
Pages: 160-163
Publication date: 2014
A model for scheduling of employees using supplier selection

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Department of Mechanical Engineering and Industrial Systems
Authors: Holopainen, S.
Number of pages: 6
Pages: 533-538
Publication date: 2014

Host publication information
Title of host publication: Engineering optimization IV, Proceedings of the International Conference on Engineering Optimization (ENGOPT 2014), Lisbon, Portugal, 8-11 September 2014
Place of publication: The Netherlands
Publisher: CRC Press/Balkema
ISBN (Print): 978-1-138-02725-1
ISBN (Electronic): 978-1-315-73210-7
DOIs: 10.1201/b17488-96

Bibliographical note
Contribution: organisation=mei,FACT1=1<br/>Portfolio EDEND: 2015-01-09
Source: researchoutputwizard
Source-ID: 491
Research output: Scientific › Conference contribution

CO-Based Outdoor Smart Lighting for Energy Aware Factory

General information
State: Published
Ministry of Education publication type: A3 Part of a book or another research book
Organisations: Department of Mechanical Engineering and Industrial Systems, Research group: Factory automation systems technology
Authors: Florea, A., Farahat, A., Postelnicu, C., Martinez Lastra, J. L., Azcondo Sánchez, F. J.
Number of pages: 15
Pages: 69-83
Publication date: 2014

Host publication information
Title of host publication: Internet of Things Based on Smart Objects
Publisher: Springer International Publishing
Editors: Fortino, G., Trunfio, P.
ISBN (Print): 978-3-319-00490-7
ISBN (Electronic): 978-3-319-00491-4
Electrically tunable localized tunneling channels in silicene nanoribbons

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Spectroscopies of Complex Materials, Department of Physics, Computational Science X (CompX)
Authors: Saari, T., Huang, C., Nieminen, J., Tsai, W., Lin, H., Bansil, A.
Number of pages: 4
Pages: 1-4
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: APPLIED PHYSICS LETTERS
Volume: 104
Issue number: 17
Article number: 173104
ISSN (Print): 0003-6951
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.132 0.996
Publication Forum (2016): 2
Scopus rating (2015): 1.085 0.983
Web of Science (2015): 3.142 3.293 7.9 0.673 0.38389 1.045
Publication Forum (2015): 2
Scopus rating (2014): 1.799 1.462
Web of Science (2014): 3.302 3.569 7.4 0.655 0.42671 1.125
Publication Forum (2014): 2
Scopus rating (2013): 2.149 1.652
Publication Forum (2013): 2
Scopus rating (2012): 2.554 1.754
Publication Forum (2012): 2
Scopus rating (2011): 2.805 1.94
Scopus rating (2010): 2.926 1.789
Scopus rating (2009): 2.857 1.848
Scopus rating (2008): 2.934 1.83
Scopus rating (2007): 3.039 1.913
Scopus rating (2005): 3.709 2.382
Scopus rating (2004): 3.904 2.38
Scopus rating (2003): 3.765 2.27
Scopus rating (2002): 3.917 2.365
Scopus rating (2001): 4.111 2.212
Scopus rating (2000): 4.277 2.013
Scopus rating (1999): 4.35 2.11
Energy efficient outdoor lighting: an implementation

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Mechanical Engineering and Industrial Systems, Research group: Factory automation systems technology
Authors: Farahat, A., Florea, A., Martinez Lastra, J. L., Branas Reyes, C., Azcondo, F. J.
Number of pages: 5
Pages: 1-5
Publication date: 2014

Host publication information
Title of host publication: 2014 IEEE 15th Workshop on Control and Modeling for Power Electronics (COMPEL), 22-25 June 2014, University of Cantabria, Santander, Spain
Place of publication: Piscataway
Publisher: The Institute of Electrical and Electronics Engineers
ISBN (Print): 978-1-4799-2147-8
DOIs: 10.1109/COMPEL.2014.6877213

Implementing KPIs for energy performance assessment in brownfield districts

General information
State: Published
Ministry of Education publication type: D3 Professional conference proceedings
Organisations: Department of Mechanical Engineering and Industrial Systems, Research group: Factory automation systems technology
Authors: Florea, A., Martinez Lastra, J. L., Marquez, J. A., Colino, A., Presser, M., Larranaga, M.
Number of pages: 21
Publication date: 2014

Host publication information
Title of host publication: Sustainable Places, October 1-3, 2014, Nice, France
Links:

Mechanical analysis of a pneumatically actuated concentric double-shell structure for cell stretching

General information
State: Published
On the Updating of Domain OWL Models at Runtime in Factory Automation Systems

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Mechanical Engineering and Industrial Systems, Research group: Factory automation systems technology
Authors: Puttonen, J., Lobov, A., Martinez Lastra, J. L.
Number of pages: 20
Pages: 46-66
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: International Journal of Web Services Research
Volume: 11
Issue number: 2
ISSN (Print): 1545-7362
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.145 0.285
Publication Forum (2016): 1
Scopus rating (2015): 0.201 0.654
Web of Science (2015): 0.257 0.44 Not Available 0.0 2.4E-4 0.192
Simulation Based Methods for Flexible Maintenance Program Development

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Mechanical Engineering and Industrial Systems, Department of Industrial Management
Authors: Aaltonen, J., Koskinen, K. T., Vainio, H., Martinsuo, M.
Number of pages: 5
Pages: 446-450
Publication date: 2014

Host publication information
Title of host publication: EuroMaintenance 2014, Congress proceedings May 5-7, Helsinki, Finland, 22nd European Congress & Expo on Maintenance and Asset Management, 6th World Congress & Global Forum on Maintenance and Asset Management
Publisher: European Federation of National Maintenance Societies
ISBN (Print): 978-952-67981-1-0

Bibliographical note
Contribution: organisation=mei,FACT1=1<br/>Portfolio EDEND: 2014-12-03<br/>Publisher name: I G I Global; Information Resources Management Association
Source: researchoutputwizard
Source-ID: 1314
Research output: Scientific - peer-review › Article

Water Hydraulics Pushes Into High-Pressure Systems

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State: Published
Ministry of Education publication type: D1 Article in a trade journal
Organisations: Department of Mechanical Engineering and Industrial Systems
Authors: Koskinen, K. T., Aaltonen, J.
Number of pages: 4
Challenges in Heterogeneous Web Data Analytics - Case Finnish Growth Companies in Social Media

Diverse data about various phenomena are implicitly available in the modern web. In particular websites categorized as social media provide rich and heterogeneous data about various entities such as people, corporations, brands as well as their properties and relationships. An analyst who seeks to leverage this diverse data is faced with the challenge of integrating and making sense of a set of heterogeneous data sources. In this paper, we provide an introduction and a problem statement for heterogeneous web data analytics. To further highlight and discuss practical challenges, we introduce a case study of Finnish growth companies in social media. Instead of a purely data-driven approach, the presented approach is rooted in the idea that an analyst can actively participate in the data collection and integration process, while the process can still retain repeatability and transparency. The key contribution of this paper is the statement of the challenges related to heterogeneous web data analytics.

General information
State: Published
Organisations: Department of Mathematics
Authors: Salonen, J., Huhtamäki, J., Nykänen, O.
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Research output: Scientific - peer-review › Conference contribution

Computational model of Ca2+ wave propagation in human retinal pigment epithelium

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Organisations: Department of Electronics and Communications Engineering, Research group: Computational Biophysics and Imaging Group
Authors: Vainio, I., Abu Khamidakh, A., Paci, M., Skottman, H., Juuti-Uusitalo, K., Hyttinen, J., Nymark, S.
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Networks of innovation relationships: multiscopic views on Finland

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Mathematics
Authors: Still, K., Huhtamäki, J., Russell, M. G., Basole, R. C., Salonen, J., Rubens, N.
Number of pages: 15
Pages: 1-15
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Process for Measuring and Visualizing an Open Innovation Platform: Case Demola
Open innovation breaks the traditional pattern for developing new innovation leading to new business and the activities toward it. Consequently, new requirements are posed to innovation measurement. Demola is an open innovation platform that takes real-life problems from companies and other organizations and puts together and facilitates projects where students from different universities come together to solve the problems. This paper describes a set of network visualizations and animations that were developed in co-creation with the Demola operators to make visible the activity that Demola has initiated. Moreover, the development process used to design the visualizations and the technical process that was applied are described and discussed. We claim that static network visualizations and animations of an open innovation platform development are useful in presenting, describing, marketing and selling the platform for existing and new stakeholders. Our experience shows that in order to develop visualizations and animations that meet the requirements set by the different stakeholders, an iterative and incremental development process is needed. Moreover, we claim that taking a data-driven approach to visualization development is a key enabler in supporting the development.

Relational Capital and Social Capital: One or two Fields of Research?

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Twiiteryhmä ja uutispäivittelyä - toimittajana sosiaalisessa mediassa

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Ministry of Education publication type: D4 Published development or research report or study
Organisations: Department of Mathematics
Authors: Vainikka, E., Noppari, E., Heinonen, A., Huhtamäki, J.
Number of pages: 113
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Verkostoanalyysi sosiaalisen median tutkimuksessa

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Authors: Huhtamäki, J., Parviainen, O.
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