19th Christmas Biophysics Workshop

Stift St. Georgen am Längsee, Austria

December 9 – 10, 2025

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Tuesday December 9

09:00	**Registration & coffee**	Check in from 15:00
09:45	**Introduction**	
	Polymers & fluids	**Chair: Tomislav Vuletić**
10:00	Pieter van der Hoek	Coherent modeling of double-folded ring polymers and their underlying random tree structure
10:15	Fran Ivan Vrban	Liquid drops meet star polymers
10:30	Ashish Kumar Singh	Effect of hydrodynamics on ring polymers under different solvent conditions
10:45	Enrico Fornasa	Emergence of giant chains in ring-linear polymer blends via efficient self-assembly Monte Carlo
11:00	Matevž Jug	Learning macroscopic equations of motion from particle-based simulations of a fluid
11:15	**Coffee**	
	Cells & tissue	**Chair: Primož Ziherl (before lunch), Antonio Šiber (after lunch)**
11:45	Ema Slejko	Developing an implicit solvation machine learning model for ionic media
12:00	Maša Lah	Open-boundary molecular dynamics of red blood cell suspensions
12:15	Jan Rozman	Why extensile and contractile tissues could be hard to tell apart
12:30	Urška Andrenšek	Surface tension-driven elasticity of circular epithelia
12:45	**Lunch**	
14:45	Toshikaze Chiba	Junctional fluctuations in three-dimensional epithelial tissue
15:00	Nives Matijaković Mlinarić	Smart antimicrobial coatings for titanium implants and biomedical textiles
15:15	James McFarlane Hoad	In vitro cytotoxicity profiles of functional coating components
15:30	Valentina Bedoya Aristizabal	Cellular noise control by out-of-equilibrium multicomponent biocondensates
15:45	Urban Železnik	Mechanics of cell aggregates as models of tumors and tumor spheroids
16:00	Bernat Corominas-Murtra	An optimum level of stochasticity in cell cycle length determines embryo morphogenesis onset
16:15	**Coffee**	
	Nanoparticles	**Chair: Giovanni Bussi**
16:45	Atida Selmani	Engineered mesoporous silica nanoparticles as lysozyme carriers
17:00	Suzana Inkret	Composite calcium phosphates/silver nanoparticles coatings on titanium
17:15	Antonio Šiber	Functionality of apertures in harmomegathy of oblate pollen grains
17:30	Nikolaos Ntarakas	Dissipative particle dynamics models of encapsulated microbubbles and nanoscale gas vesicles
17:45	Fabio Staniscia	Interfacial properties of nanodroplets and nanobubbles
18:00	Silvia Tomić	Tribute to Rudi Podgornik
19:00	**Dinner**	
21:00	Various contributors	Session dedicated to Rudi Podgornik

Wednesday December 10

07:30	**Breakfast**	Check out before 10:00
	Lipids & surfactants	**Chair: Douwe Jan Bonthuis**
09:00	Helena Biljanić	Assessment of fatty acid biocompatibility in endothelial cells for biomedical applications
09:15	Matej Kanduč	How trees suck water 100 meters high without cavitation?
09:30	Katarina Kokalj	Simulating rupture: molecular dynamics insights into ultra-thin surfactant film instability
09:45	Saša Svetina	On the effects of differential stress on properties of lipid bilayers
10:00	Michael Kaltenegger	Establishment and construction of a confocal single-molecule microscope
10:15	Ivana Ruseska	Transfection-induced modulation of cell membrane roughness
10:30	**Coffee**	
	DNA, RNA & proteins	**Chair: Cristian Micheletti**
11:00	Nataša Holler	GLP-1 receptor-mediated targeted drug delivery in 3T3-L1 fibroblasts
11:15	Veronika Bukina	Long-range base-pairing interactions underlying the compact structure of viral RNA genomes
11:30	Moritz Smilde	Quantitative prediction of protein allostery
11:45	Fraser MacMillan	Exploring structural and mechanistic dynamics of macromolecules with magnetic resonance
12:00	Domen Vaupotič	Detection and classification of low-complexity RNA sequences
12:15	Maurizio Gilioli	Using molecular dynamics to characterize influenza a ribonucleoproteins' dynamics
12:30	Alessandro Piras	Plectoneme translocation
12:45	**Lunch**	

Surface tension-driven elasticity of circular epithelia

U. Andrenšek[1,2] and M. Krajnc[2]
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[2]Jožef Stefan Institute, Ljubljana, Slovenia

During the life of animals, epithelial tissues undergo extensive deformations–first to form organs during embryogensis and later to preserve integrity and function in adulthood. To what extent these deformations resemble that of non-living elastic materials is not well understood. We derive an elasticity theory of a circular epithelia, in which the mechanics of individual cells are dominated by differential interfacial tensions stemming from cell cortical tension and adhesion. We observe a critical value of differential surface tension at which the tissue spontaneously wrinkles. We derive the critical force to induce the wrinkling instability and its dominant deformation mode, where the apico-basal symmetry is broken by both the differential surface tension and the radius of the circular tissue.

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Cellular noise control by out-of-equilibrium multicomponent biocondensates

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Cells must reliably regulate gene expression despite substantial intracellular fluctuations. Stochasticity in transcription and translation generates high variability in protein concentrations, yet cells achieve robust function through mechanisms that buffer these fluctuations. Biomolecular condensates (Biocondensates) formed by liquid-liquid phase separation provide one such mechanism: by dynamically partitioning molecules between dilute and dense phases, condensates help maintain the free-particle concentration fluctuations within a narrow range even when total molecular copy numbers vary. Experiments and theory have demonstrated noise reduction in single-component condensates under near-equilibrium conditions.

However, endogenous condensates are inherently multicomponent and operate far from equilibrium due to molecular turnover, active processes, and compositional regulation. How these features jointly influence noise control remains poorly understood, and a framework that simultaneously accounts for multicomponent thermodynamics and non-equilibrium kinetics is still lacking.

In this work, we develop a theoretical and computational approach to quantify fluctuations in out-of-equilibrium multicomponent Biocondensates. We combine condensates thermodynamics with stochastic kinetics and use a system-size-expansion approach to quantify mean concentrations and their fluctuations. This framework lays the groundwork for a unified description of how compositional complexity and non-equilibrium activity shape the noise-buffering capabilities of cellular condensates.

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Assessment of fatty acid biocompatibility in endothelial cells for biomedical applications

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[1]Ruđer Bošković Institute, Zagreb, Croatia
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Fatty acids (FAs) represent a diverse group of molecules in which chain length and degree of saturation determine their physicochemical properties and biological behaviour. Depending on their structure, FAs elicit distinct cellular responses: saturated FAs can promote pro-inflammatory signaling and cytotoxicity, while polyunsaturated FAs display anti-inflammatory effects and inhibit monocyte adhesion. Owing to these differences, understanding which types of FAs are suitable for specific biomedical applications, such as reducing inflammation, improving implant integration or achieving sustained drug release. This study quantitatively investigates the biocompatibility and cytotoxicity of selected saturated (octanoic, stearic, behenic) and unsaturated (elaidic, oleic, linoleic) FAs using the human endothelial cell line Ea.hy926. The results reveal correlations between molecular structure and cellular response, offering insight into the biophysical mechanisms that govern cell interactions with FAs. Applying these findings to the metal implant surface could improve corrosion resistance, regulate inflammatory responses, and enhance material stability and performance in biomedical applications.
This work was supported by the Croatian Science Foundation (HRZZ MOBDOK-2023-7329).

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Identification of long-range base-pairing interactions underlying the compact structure of viral RNA genomes

V. Bukina[1,2], D. Vaupotič[1,2], A. Božič[1]
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RNA structure plays a central role in viral replication, gene expression, and genome packaging, with many single-stranded RNA (ssRNA) viruses evolving unusually compact conformations to fit within small icosahedral capsids. This compactness can be quantified through the ensemble-averaged maximum ladder distance (MLD), which is consistently lower in wild-type viral genomes than in randomized or synonymously shuffled sequences. To probe the mutational limits of this property, we apply a directed synonymous-mutation evolutionary algorithm to three +ssRNA viruses – Brome Mosaic Virus (BMV), Blueberry Shock Virus (BlShV), and Beet Virus Q (BVQ) – while preserving nucleotide, dinucleotide, and codon composition. Mutants are evaluated via Boltzmann-sampled secondary structures, and those with extreme MLD are iteratively selected using a Metropolis-enabled search. Our results show that compact viruses such as BlShV have little remaining flexibility to further reduce MLD, whereas BVQ can be driven toward more compact or more extended folds. Arc-based structural analyses identify specific interaction motifs governing these shifts, illustrating how synonymous mutations can modulate RNA architecture within evolutionary constraints.

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Junctional fluctuations in three-dimensional epithelial tissue

Toshikaze Chiba and Matej Krajnc
Jožef Stefan Institute, Ljubljana, Slovenia

During embryogenesis, cell rearrangements drive epithelial tissue deformation. Particularlly in three-dimensional space, it remains unclear how asymmetric forces between apical and basal surfaces play a role in cell rearrangements. In this study, we investigated cell rearrangements using a graph-vertex-model with asymmetric conditions driven by active forces. We analyzed diffusion processes of cell displacement over long time scales by introducing fluctuations to junctional tension. On diffusion processes, we also inspected the effects of topological changes such as scutoids and delamination. Together, our results suggest a possible scenario for rigidity transitions driven by junctional and motility fluctuations in three dimensional epithelial tissues, which more closely resemble actual biological conditions.

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An optimum level of stochasticity in cell cycle length determines the onset of embryo morphogenesis

Bernat Corominas-Murtra[1], Adrián Aguirre-Tamaral[1], Magdalena Schindler[2] and Nicoletta Petridou[2]
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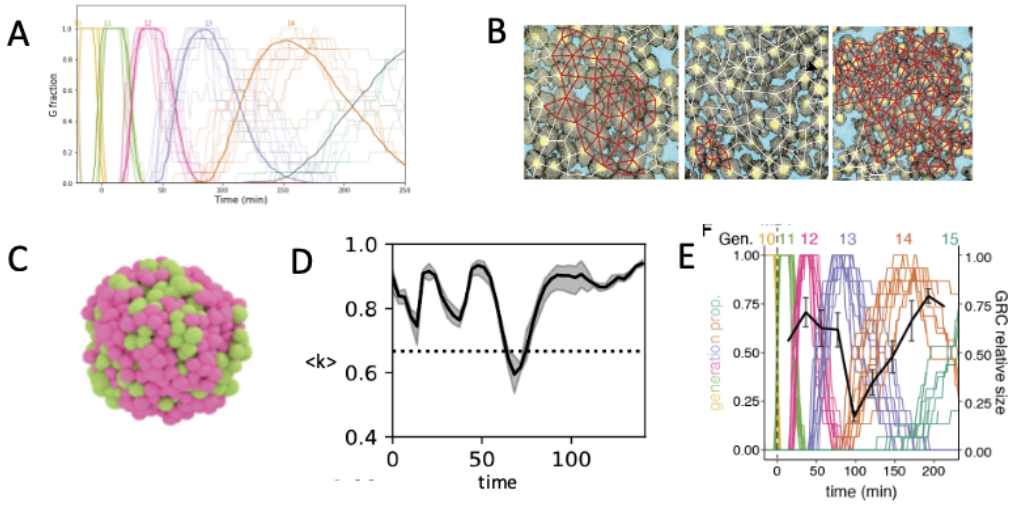
During embryogenesis, cells operate collectively yet display pronounced physiological heterogeneity. Whether this cell-level disorder is merely buffered or harnessed to drive morphogenesis remains unclear. We will show that an optimum degree of stochasticity in cell division timing determines the onset of embryo-scale morphogenesis. By combining quantitative cell-lineage tracking with mechanical rigidity frameworks in zebrafish, we find that the onset of morphogenesis – marked by a collapse of tissue rigidity – occurs precisely when variability in cell cycle length peaks. Surprisingly, one can show both mathematically and experimentally that cell cycle heterogeneity arises not from random biological noise, but from size-dependent stochasticity in resource allocation that is inherited and amplified across generations. This heterogeneity accumulates through generations and couples with the explosive, hyperbolic growth of the cell cycle length. By integrating theory of stochastic processes, in vivo experiments and large-scale 3D simulations, we show that tuning cell cycle variability alone is sufficient to coordinate global contact remodelling and drive robust, tissue-level mechanical transitions. Overall, these findings demonstrate how multicellular systems exploit an interplay between deterministic constraints and biological noise to optimally fine-tune cellular stochasticity and drive collective behaviour during morphogenesis.



A/ Generation rounds through time, solid lines theory, rugged lines experiment B/ Collapse of the rigid cluster at the onset of morphogenesis (in red) C/ In-silico cell mass, different colors different generations, D/ Crossing the critical point in connectivity <k> once at the onset of morphogenesis (simulation) and E/ collapse of the rigid cluster across generations

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Emergence of giant chains in ring-linear polymer blends via efficient self-assembly Monte Carlo

Enrico Fornasa
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Fixed-composition polymer melts are hard to equilibrate by molecular dynamics or Monte Carlo, as wall-clock decorrelation times typically grow at least quadratically with chain length, N. Here, we introduce a self-assembly Monte Carlo (SAMC) scheme that uses end-point bond swaps to evolve fully packed ring-linear blends while preserving self-avoidance, density, and the number of linear chains, n. The move provides a uniform stationary measure over the self-assembly ensemble of composition-unrestricted blends and avoids backbone tracing. As a result, the global wall-clock decorrelation time scales quasi-linearly with volume, $\sim V^{1.07}$. Notably, the self-assembly ensemble supports the emergence of giant linear chains that are individually macroscopic and collectively occupy ≈90% of the volume, while the background rings remain finite and non-extensive. Combined with the efficient decorrelation of SAMC, this enables routine sampling of systems with chains of $\sim 10^6$ monomers. The giant chains have melt-like metric statistics, and hence we use them to characterize linear melt properties, such as intra- and inter-chain entanglements, in density and length regimes not previously addressed. We find that both knotting and linking occur at localized and widely separated regions and additionally show that the Gauss linking integral of neighboring chains grows only as $N^{1/4}$. SAMC thus offers an efficient strategy for sampling fully packed lattice polymers in contexts where emergent giant components open previously unexplored density and size regimes.

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Using molecular dynamics to characterize influenza a ribonucleoproteins' dynamics

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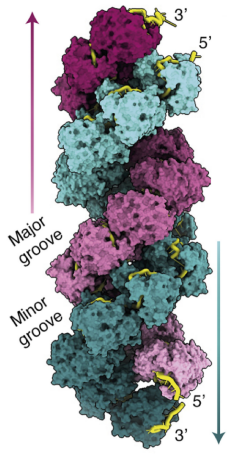
Influenza A viruses are pathogens responsible for human seasonal epidemics and severe animal pandemics. Their genome consists of eight RNA segments, each packaged into a ribonucleoprotein complex (RNPs). During co-infection of a host cell by different strains of influenza virus, the RNPs can be exchanged or "shuffled" between viruses, leading to progeny viruses that contain a mixture of RNA segments from the parental strains. This event enables rapid evolution and emergence of new viral strains with mixed traits. Reassortment requires correctly assembled RNPs, which helps explain why their architecture is so highly conserved. This conservation makes RNPs appealing targets for broad-spectrum antivirals and for structural analysis. Despite substantial prior work, most studies focused on the characterization of single NP monomers. Only recently, advancements in Cryo-EM enabled researchers to resolve the complete structure of an influenza A RNP, at an overall resolution of 3.2 Å. Nevertheless, these structures are averaged over multiple experimental particles, lack some unresolved regions, and are obtained using truncated viral RNAs. In this work, we first reconstruct the unresolved regions of a RNP complex and then employ molecular dynamics (MD) simulations to quantify the dynamical fluctuations of an RNP monomer both in isolation and within an asymmetric unit containing neighboring monomers. The resulting dynamics is compared with available Cryo-EM data.



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GLP-1 receptor-mediated targeted drug delivery in 3T3-L1 fibroblasts

Nataša Holler[1], Bernd Gesslbauer[1], Ilse Letofsky-Papst[2], Claudia Mayrhofer[2] and Andreas Zimmer[1]
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The development of nanocarriers for targeted drug delivery is currently one of the largest

fields in pharmaceutical research. The focus of our research is on peptide-directed nanoemulsions (NEs). As model substance, a 39 amino acids long GLP-1 receptor agonist, exendin-4, is used. In a click-chain reaction, exendin-4 is coupled via a PEG linker to a phospholipid, thereby enabling the attachment of the peptide to the surface of the oil droplets within the nanoemulsion. The raw nanoemulsion, which served as the formulation base, was prepared using high-pressure homogenization. Subsequently, it was mixed with the peptide conjugate to prepare a peptide-directed nanoemulsion. The functionality of the drug carrier is tested on 3T3-L1 mouse fibroblasts, which are a commonly used tool for study of the subcellular pathways involved in preadipocytic cell differentiation [1]. Our findings demonstrate that uptake rates were higher when the peptide was present on the surface of the oil droplets compared to control. This tendency is even more pronounced after the fibroblasts are fully differentiated to the mature adipocytes. This suggests a specific or a receptor-mediated uptake. In subsequent studies, we intend to investigate the impact of varying concentrations of the peptide per oil droplet and to compare the uptake dynamics in different cell lines.

[1] Dufau, J., Shen, J. X., Couchet, M., de Castro Barbosa, T., Mejhert, N., Massier, L., Griseti, E., Mouisel, E., Amri, E. Z., Lauschke, V. M., Ryden, M., & Langin, D, In vitro and ex vivo models of adipocytes. American Journal of Physiology - Cell Physiology 2021, 320(5), 822–841.

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Composite calcium phosphates/silver nanoparticles coatings on titanium – a possible way of improving titanium implants properties

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[3]Innovations Institute for Nanotechnology and Correlative Microscopy, INAM, Forchheim, Germany

Titanium and its alloys are widely used as implant materials for hard tissues due to their excellent chemical inertness, mechanical stability, and biocompatibility [1]. However, two major challenges persist in their application: insufficient integration of implants with surrounding tissues and a high risk of infections. Surface modification and functionalization with calcium phosphate (CaP) coatings enhance osseointegration, while the incorporation of silver nanoparticles (AgNPs) provides antimicrobial properties [2]. In this study, titanium surfaces were chemically modified using two acid etching methods: a soft method (HCl) and a more aggressive one (H2SO4/HCl) [3,4]. CaP/AgNP coatings were prepared by wet chemistry method. The influence of different etching methods and coatings on roughness, wettability, morphology and overall, surface coverage with coatings was investigated. Etching altered key surface features, including roughness and wettability. On both types of surfaces, AgNPs were formed. CaP/AgNP composite coatings improved hydrophilicity, to varying degrees depending on the etching method.Surface coverage also depended on the etching method, and it was better with more aggressive etching. These results demonstrate that controlled surface modification of titanium is crucial for optimizing coating deposition and enhancing titanium implants' properties, enabling in that way implants' performance in biomedical applications. Keywords: calcium phosphates, silver nanoparticles, titanium implants. Acknowledgement: Financial support from Croatian Science Foundation, Grant HRZZ-DOK-2021-02-5447 and MOBDOK-2023-4472.

[1] X. Lu, Z. Wu, K. Xu, X. Wang, S. Wang, H. Qiu, X. Li, J. Chen, Front. Bioeng. Biotechnol., 9 (2021) 783816
[2] S.L. Percival, P.G. Bowler, D. Russell, J. Hosp. Infect., 60 (2005) 1–7
[3] X. Lu, Z. Zhao, Y. Leng, Mater. Sci. Eng. C, 27 (2007) 700–708
[4] D. Wang, G. He, Y. Tian, N. Ren, W. Liu, X. Zhang, J. Biomed. Mater. Res., 108 (2020) 2386–2395

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Learning macroscopic equations of motion from particle-based simulations of a fluid

Matevž Jug[1,2], Daniel Svenšek[1,2], Tilen Potisk[1,2], and Matej Praprotnik[1,2]
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Describing the dynamics of a material in terms of partial differential equations provides a systematic framework for predicting its behavior on large spatio-temporal scales, which are suitable for engineering applications. However, for novel complex materials, only a particle-based description is usually available. Since simulations of these particle-based models can generate vast amounts of data, the discovery of dynamic equations through data-driven means is becoming increasingly popular. The method that will be presented combines a weak formulation of the unknown equations, sparse regression (specifically, the SINDy [1] framework), and a new model selection measure that balances stability and accuracy to discover equations governing continuum-level dynamics directly from particle-based simulations [2]. From simulations of a simple fluid, modeled using dissipative particle dynamics, our method successfully extracts the mass continuity equation and the Navier-Stokes equation, the latter also containing the correct equation of state. Due to its high robustness to noise, such an approach can be readily applied to simulations or experimental data of more complex materials, where macroscopic dynamic equations are not, or are only partially, known.

[1] Brunton, S. L., Proctor, J. L., Kutz, J. N., Proc. Natl. Acad. Sci. USA 113, 3932 (2016)
[2] Jug, M., Svenšek, D., Potisk, T., Praprotnik, M., Comput. Methods Appl. Mech. Eng. 432, 117379 (2024)

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Establishment and construction of a confocal single-molecule microscope

Michael Kaltenegger, Georg Krainer and Georg Pabst
Institute of Molecular Biosciences, University of Graz, Austria

The elastic properties of lipid bilayers and their possible influence on transmembrane proteins are of great interest in the field of membrane biophysics. In particular, total internal reflection microscopy(TIRF) was employed to investigate protein-protein interactions in single molecule Förster resonance energy transfer(smFRET)-studies. However, TIRF-measurements require the immobilization of the observed system onto functionalized microscopy coverslip. This tethering and the proximity to the glass surface may alter the

elastic properties of the lipid structures. To circumvent this problem, we opted to employ confocal single molecule studies with the advantage of carrying out measurements in solution and thereby preserving the native properties of the lipid systems. As part of this project, we successfully planned out and constructed a single molecule confocal setup and started validation- and calibration-measurements. For this purpose, we designed fluorescently labelled DNA-constructs, including FRET-rulers and hairpin structures. The DNA-rulers exhibit three different FRET-states, while hairpin structures demonstrate dynamic transitions between states. Measurements of the above-mentioned designs showcase the abilities of the system to distinguish between static FRET-states and detect dynamic behaviour. After further optimization, the setup will be used to examine more complex biological systems, with a particular focus on, but not limited to, lipid-protein interactions.

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How trees suck water 100 meters high without cavitation?

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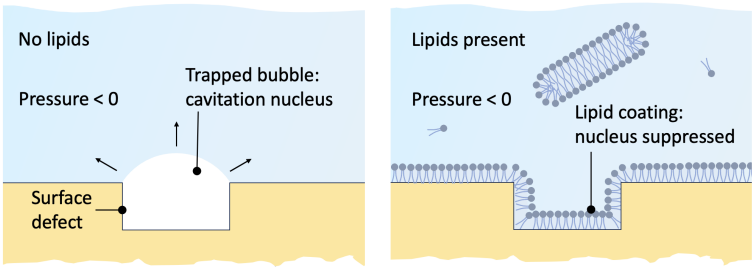
With enough care, water can be prepared to withstand stretching – that is, to sustain tension or negative pressure – before it finally cavitates by forming bubbles. But this only works when the water is exceptionally clean. It therefore comes as a surprise that plant sap, which flows under substantial negative pressures of up to -100 atm, is anything but clean. It contains ions, sugars, lipids, and all sorts of organic molecules that should, in principle, make it more prone to cavitation – and yet, plants transport water reliably over long distances. Using a multiscale approach that combines molecular simulations with classical nucleation theory, we found that amphiphilic molecules, such as lipids, may actually be part of the solution. By adsorbing onto tiny hydrophobic crevices, they can "passivate" sites that would otherwise trap nanobubbles and trigger cavitation. In doing so, they help water remain intact even under extreme tension. Nature's trick is not to keep water pure, but to protect it.



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Simulating rupture: molecular dynamics insights into ultra-thin surfactant film instability

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[2]Faculty of Mathematics and Physics, University of Ljubljana, Slovenia.

Ultra-thin surfactant films are central to many systems, including foams, emulsions, and soft interfaces, yet the molecular origins of their instability and sudden rupture remain difficult to capture experimentally. Rupture is generally initiated once a thermally nucleated pore exceeds a critical size, a process that can be framed within classical nucleation theory. To investigate this process in detail, we employ molecular dynamics simulations using GROMACS to follow pore formation and subsequent film failure. Our simulations show that the rupture behavior is comparable in films with and without a separating water layer, implying that interfacial characteristics, such as surfactant packing and the edge tension, dominate over solvent contributions. Differences in rupture propensity across systems can be traced to variations in edge tension and to the presence of H-bond networks within the surfactant monolayers. These molecular-scale features provide practical levers for tuning the stability of ultra-thin films for targeted applications.

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Effect of hydrodynamics on ring polymers under different solvent conditions

Ashish Kumar Singh and Angelo Rosa
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We consider single-ring and multiple-ring systems and compare their static and dynamical properties, by using Molecular Dynamics computer simulations with explicit solvent. By switching from good- to bad-solvent conditions, we show that the two types of systems react quite differently, in particular systems with multiple chains tend to be dynamically stuck. We argue that the reported behavior is caused by ring-ring interpenetrations, and characterize this behavior by a detailed analysis of static and dynamic properties.

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Open-boundary molecular dynamics of red blood cell suspensions

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Blood is a complex suspension of deformable red blood cells whose collective behavior governs bulk rheology and affects physiological function. Although numerous computational studies have simulated blood flow, most rely on periodic boundary conditions, which cannot reproduce realistic mass and momentum exchange essential for non-equilibrium pro-

cesses. Open-boundary molecular dynamics (OBMD) is a particle-based framework that overcomes this limitation by explicitly controlling fluxes across open boundaries. While OBMD has demonstrated success in simulating complex systems, it has not yet been applied to homogeneous suspensions. In dense suspensions, inserting large objects, which is a key feature of OBMD's mass exchange, is challenging due to limited space. We extend OBMD to red blood cell (RBC) suspensions using a novel growing-size membrane insertion algorithm that enables simulations at physiologically relevant high hematocrits while preserving bulk hemorheology, including shear-thinning and hematocrit-dependent viscosity [1]. This framework establishes a foundation for future studies of acoustically driven RBC suspensions.

[1] M. Lah, T. Potisk, and M. Praprotnik, Open-boundary molecular dynamics of red blood cell suspensions, submitted.

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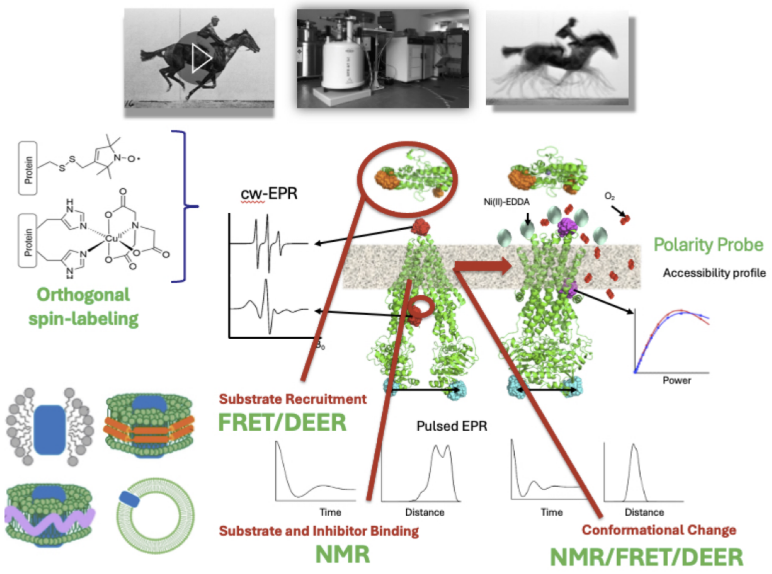
Exploring structural and mechanistic dynamics of macromolecules with magnetic resonance

Fraser MacMillan
Institut za fiziku, Bijenička Cesta 46, 10000 Zagreb, Croatia

This research focuses on the architecture and functional dynamics of membrane proteins, many medically relevant with a special interest on membrane transport. There is increasing evidence that membrane proteins don't act alone but are organised as nano-machineries which function through the concerted action of their individual components with high precision and specificity observed in both time and space. We seek to unravel the principles underlying the architecture, dynamics and ultimately function of these protein nano-machineries using advanced magnetic resonance techniques, specifically pulsed Electron Paramagnetic Resonance (EPR) – but also NMR techniques in combination with molecular biological and other biophysical methods. Our expertise lies in the development and application of novel techniques to address key questions.

Here I will focus on recent method developments, which allow a shifting of the focus of magnetic resonance from being considered purely a niche technique towards a more universal structural biological tool. I will demonstrate, e.g., how to resolve multiple distance constraints in macromolecular ensembles, how to observe dynamic conformational changes at the molecular level and finally to identify the dynamic determinants of ligand binding.

Research has been funded by The Royal Society, BBSRC and the Wellcome Trust as well as EU MCSA ETN 'NeuroTrans'.



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Luminescent insulin-Au(III) conjugate – structure and biological function

Ž. Sanader Maršić[1,2], D. Maysinger[3], I. Zhang[3], H. Yuan[4], V. Bonačić-Koutecký[2] and R. Antoine[4]

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[2]Center of Excellence for Science and Technology, Integration of Mediterranean Region (STIM), Faculty of Science, University of Split, Croatia

[3]Department of Pharmacology and Therapeutics, McGill University, Canada

[4]Institut Lumière Matière, CNRS UMR 5306, Université Claude Bernard Lyon 1, France

We report on the structural characterization and nonlinear optical properties of insulin-gold conjugates. Such conjugates display strong luminescence at ∼670 nm. By combining experimental studies and time-dependent density functional theory simulations (TD-DFT), we show the formation of insulin-Au(III) conjugates [1]. Further, we wanted to establish if insulin conjugated with auric gold Au(III) can be visualized in living cells expressing insulin receptors, and if key steps in insulin signaling are undisturbed. Au(III) is coordinated with three tyrosines of insulin and is strongly stabilized by coordination with these tyrosines into a metal-ion coordinated insulin template. We combined theoretical and experimental approaches to analyze the cellular effects of this construct. Results show that the insulin-Au(III) conjugate does not impair several steps in insulin signaling and downstream metabolic functions in lysosomes and lipid droplets [2]. The luminescent properties of insulin-Au(III) could serve to combine biochemical and imaging studies in human cells beyond microglia.

[1] D. Bain et al., One- and two-photon brightness of proteins interacting with gold. A closer look at gold-insulin conjugates, Nanoscale, 2024, 16, 14953-14958

[2] D. Maysinger et al., Luminescent insulin-Au(III) conjugate retains insulin biological properties in human microglia, Nanoscale, 2025, 17, 16806-16817

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Smart antimicrobial coatings for titanium implants and biomedical textiles: balancing biocompatibility and infection control

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Microbial infections associated with biomedical interfaces, including implants, textiles, and high-touch surfaces, remain a significant clinical challenge, particularly against biofilm-forming pathogens such as Staphylococcus aureus (S. aureus), Staphylococcus epidermidis (S. epidermidis), and Escherichia coli (E. coli). Possible strategies to explore antimicrobials include metal ion or nanoparticle-functionalized polyelectrolyte coatings and bioactive mineral layers applied to textiles, stainless steel, and titanium. In this study, ZnO and CuO nanoparticles of various sizes and morphologies, along with Zn^{2+} ions, were incorporated into polyelectrolyte coatings on various surfaces. The results demonstrated that ZnO nanoparticles immobilized in poly(allylamine hydrochloride) and alginate multilayers produced strong antibacterial performance, achieving 2-3 log (>99%) reduction of S. aureus on coated textiles, while released Zn^{2+} concentrations remained well below cytotoxic limits (7-10 μg mL^{-1}), preserving keratinocyte viability [1]. Stainless steel surfaces functionalized with poly(allylamine hydrochloride) and alginate and ZnO or CuO nanoparticles achieved complete eradication of E. coli, with ZnO demonstrating superior efficacy, while both systems remained cytocompatible due to controlled ion release [2]. On titanium, $ZnO/CaCO_3$ (vaterite) composite coatings achieved >90% viability reduction for S. aureus, S. epidermidis, and Candida albicans, while maintaining Zn^{2+} release below cytotoxic thresholds for osteoblast cells [3]. In conclusion, polyelectrolyte-immobilized ZnO, $ZnO/CaCO_3$ mineral coatings, and controlled CuO systems demonstrated an effective balance of antimicrobial potency and biocompatibility for application on various biomedical surfaces.

[1] Matijaković Mlinarić, N., et al., Nanomaterials 14 (2024), 570

[2] Matijaković Mlinarić, N., et al. ACS Appl Nano Mater 7 (2024) 12550-12563

[3] Selmani, A., et al. J Funct Biomater 16 (2025), 108.

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In vitro cytotoxicity profiles of functional coating components for high-performance protective fabrics

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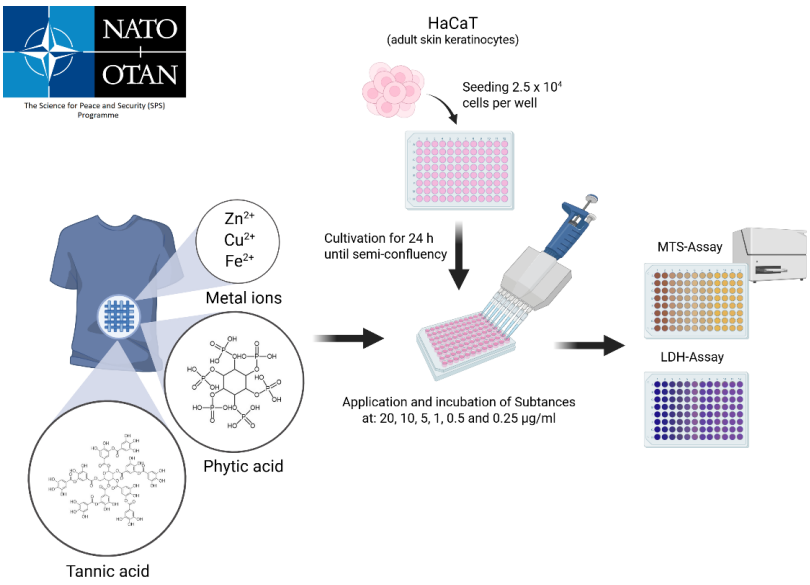
The SAFEGUARD project aims to develop secure, antibacterial, UV-protective, and flame-

retardant textiles for use in military uniforms, protective gear, shelters, field hospitals, medical kits, and related civilian applications. These multifunctional materials are engineered through coatings containing metal ions (Zn^{2+}, Cu^{2+}, Fe^{3+}) combined with tannic acid and phytic acid to impart durable protective properties. To ensure safe skin contact and assess potential risks from component leaching, the cytotoxicity of each coating constituent was evaluated using HaCaT adult human skin keratinocytes. Cells were exposed to 0.25-20 μg/mL for 4 hours, followed by quantification of mitochondrial activity (MTS assay) and membrane integrity (LDH release assay). Zn^{2+} exhibited no cytotoxicity up to 5 µg/mL. In contrast, C^{2+} and Fe^{3+} induced concentration-dependent effects at $\geq$5 μg/mL, with C^{2+} causing a notable reduction in viability (<60%) and Fe^{3+} producing only a mild decrease (60-80%). Phytic acid was well tolerated up to 10 μg/mL, whereas tannic acid reduced viability at concentrations as low as 1 μg/mL. These findings provide clear, component-specific safety profiles that will guide the development of high-performance protective textiles with minimized risk for end-users.



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Dissipative particle dynamics models of encapsulated microbubbles and nanoscale gas vesicles for biomedical ultrasound simulations

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[1]Laboratory for Molecular Modeling, National Institute of Chemistry, Ljubljana, Slovenia

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[3]Institute of Complex Systems (UBICS), Universitat de Barcelona, Barcelona, Spain

Ultrasound-guided drug and gene delivery (USDG) enables controlled and spatially precise delivery of drugs and macromolecules, encapsulated in microbubbles (EMBs) and gas vesicles (GVs) to target areas such as tumors. It is a non-invasive, high-precision, low toxicity process with significantly reduced drug dosage. The outcome of USDG and imaging is strongly influenced by the rheological and acoustic properties of GVs and EMBs, making detailed modeling of their physical properties pivotal for ultrasound-mediated therapeutic applications. State-of-the-art shelled bodies continuum models cannot capture key features

such as varying shell thickness, interactions with surrounding solvents, or chemical surface functionalizations, which are vital for GV-blood interactions tuning. Our general particle-based modeling framework for encapsulated bodies accurately captures their elastic and rheological behavior at mesoscopic and nanoscale levels. Using dissipative particle dynamics, we model the solvent, gas phase of the capsid, and triangulated surfaces of immersed objects. Their elastic response is validated through stretching, buckling and shear flow simulations, eigenmode analysis, and the predicted GV buckling pressure is compared with experimental data. This approach paves the way for large-scale simulations of encapsulated bodies of various shapes and local anisotropy, capturing their dynamics, interactions, and collective behavior.

[1] Ntarakas, N., et al. Dissipative particle dynamics models of encapsulated microbubbles and nanoscale gas vesicles for biomedical ultrasound simulations. ACS Appl. Nano Mater. 2025, 8, 16053-16070

back to the program

Plectoneme translocation

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The translocation of DNA through pores of nanoscale dimensions is important in both biological processes in vivo and in single-molecule experimental setups. Experimental measurements of ionic current traces in voltage-driven translocations of DNA have recently detected the emergence of two distinct structural motifs: knots and plectonemes. The latter are twisted structures induced by the propagation of torsion originating from the electro-osmotic flow in the pore region. We studied plectoneme formation using molecular dynamics simulations in LAMMPS with a coarse-grained DNA model by Chirico and Langowski, where a DNA filament is coarse-grained as a twistable chain of beads. We performed simulations at different values of applied torque and force to study how the translocation time, number, and length of plectonemes depend on these factors.

back to the program

Why extensile and contractile tissues could be hard to tell apart

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Active nematic models explain the topological defects and flow patterns observed in epithelial tissues, but the nature of active stress – whether it is extensile or contractile, a key parameter of the theory – is not well established experimentally. Individual cells are contractile, yet tissue-level behavior often resembles extensile nematics [1,2]. To address this discrepancy, we use a continuum theory with two-tensor order parameters that distinguishes cell shape from active stress. We show that correlating cell shape and flow, whether in coherent flows in channels, near topological defects, or at rigid boundaries, cannot unambiguously determine the type of active stress [3]. Our results demonstrate that

simultaneous measurements of stress and cell shape are essential to fully interpret experiments investigating the nature of the physical forces acting within epithelial cell layers.

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[2] G. Duclos, C. Blanch-Mercader, V. Yashunsky, G. Salbreux, J.-F. Joanny, J. Prost, and P. Silberzan, Nat. Phys. 14, 728 (2018)
[3] J. Rozman, S. P. Thampi, and J. M. Yeomans, arXiv:2511.07012 (2025)

back to the program

Transfection-induced modulation of cell membrane roughness

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Nanoparticle-mediated delivery of nucleic acids can induce subtle biophysical changes in target cells, yet the effects on cellular surface topography remain largely unexplored [1]. Here, we investigated the impact of cationic nanostructured lipid carriers (cNLCs) and protamine-based nanoparticles (proticles) as miRNA delivery systems on the membrane and nuclear roughness of 3T3-L1 cells. Cells were transfected with either proticles or cNLCs, incubated for 4 hours, and fixed for atomic force microscopy (AFM) imaging. Topographic images were analysed using Gwyddion to quantify surface roughness via root mean square (Rq) values. Proticle treatment selectively increased membrane roughness, suggesting localized perturbation of the plasma membrane during internalization. In contrast, cNLCs induced a pronounced increase in nuclear roughness, indicating enhanced perinuclear actomyosin tension (Figure 1). There results indicate that nanoparticle composition distinctly modulates cellular topography. Moreover, the data imply that each nanoparticle type is taken up and trafficked differently within the cells. These AFM findings align with prior studies indicating that cNLCs more effectively disrupt endosomes than proticles, potentially explaining the greater nuclear roughness observed.

[1] Lee, C.-W., Jang, L-L., Pan, H-J., Chen, Y.-R., Chen, C.-C., Lee, C.-H. Membrane roughness as a sensitive parameter reflecting the status of neuronal cells in response to chemical and nanoparticle treatments. J. Nanobiotechnol.,14 (2016)

back to the program

Engineered mesoporous silica nanoparticles as lysozyme carriers for enhanced antibacterial & wound healing potential

A. Selmani[1], C. Iriarte Mesa[2], N. Matijaković Mlinarić[3], L. Vergeiner[1], J. McFarlane Hoad[1], R. Jeitler[1], L. Seidl[2], F. Kleitz[2] and Eva Roblegg[1]
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Mesoporous silica nanoparticles (MSNs) have emerged as versatile nanocarriers due to their high surface area, tuneable pore structure, ease of surface functionalization and biocompatibility. These properties enable efficient drug loading, protection, and controlled release, making them ideal platforms for therapeutic applications. In this study, two MSN morphologies, rod- and dendritic-like were synthesized. The resulting materials were functionalized with phosphonate and amino groups [1] to evaluate how surface chemistry and surface charge affect interactions with lysozyme. Lysozyme immobilization was performed using two approaches, depending on the surface chemistry. For calcined and phosphonate-functionalized MSNs, lysozyme was incorporated via physical adsorption, whereas for amino-functionalized MSNs, lysozyme entrapment was achieved through a glutaraldehyde-mediated reaction. The results demonstrated that morphology, surface chemistry and charge and the immobilization method influence enzyme loading and antibacterial activity. Dendritic MSNs exhibited stronger antibacterial effects against S. aureus, a bacterium highly relevant to wound infections, compared to rod-like MSNs. Furthermore, phosphonate-functionalized MSNs showed the most pronounced antibacterial performance relative to the calcined and amino-functionalized samples, indicating more favorable enzyme-surface interactions due to their surface charge. These findings highlight the important role of surface functionalization and immobilization techniques in optimizing MSN-based enzyme carriers for antibacterial and wound healing applications.

[1] C. Iriarte-Mesa et al., Functionalization of Silica Nanoparticles for Tailored Interactions with Intestinal Cells and Chemical Modulation of Paracellular Permeability. Small Sci. 2025, 5, 2400112. Doi: 10.1002/smsc.202400112.

back to the program

Interfacial properties of nanodroplets and nanobubbles

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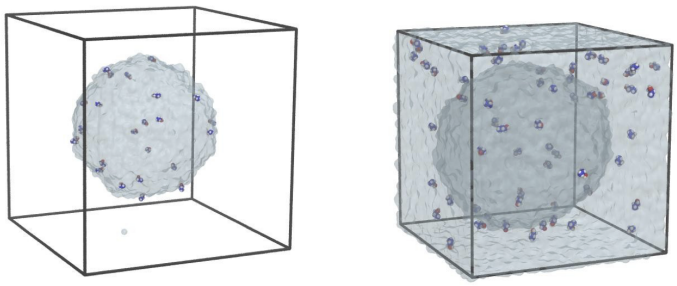
The interfaces of nano-sized droplets and bubbles are much more curved than those of macroscopic liquids, and their properties have remained elusive and largely unexplored, primarily due to challenges in direct experimental observation. In this talk, I will show how molecular dynamics simulations help us getting insights on the differences between the interfaces of nano-systems and those of macroscopic systems. We characterize the dependence of surface tension on curvature on pure systems, like water, and on solutions of surfactants in water. Since surfactants are molecules that adsorb to interfaces and reduce surface tension, we show that also their adsorption properties systematically depend on curvature. For the systems investigated, adsorption is enhanced on droplets and reduced on bubbles, with the effect becoming more pronounced for surfactants with longer hydrophobic tails. We investigate this phenomenon also in droplets deposited on a substrate. Here surfactants can also be adsorbed at the other interfaces (water-substrate and the vapor-substrate), and at the three-phase contact line. These results have broad implications across various fields, from cloud formation and climate modeling to the stability and reactivity of nanodroplets and nanobubbles.



Simulation snapshots of a droplet (left) and a bubble (right). Surfactants (in this case propanol) are shown in all-atom representation, while water is represented as a transparent smoothed density isosurface.

back to the program

Functionality of apertures in harmomegathy of oblate pollen grains

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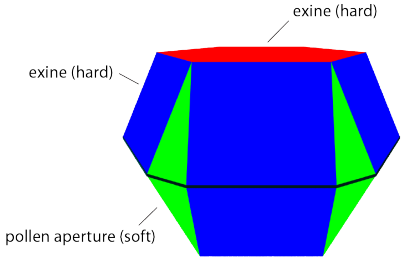
The effectiveness of pollen apertures in guidance of harmomegathy – the change in the shape of pollen grains to prevent their dehydration – has so far been investigated in spherical [1] and prolate [2] pollen grains. Of all pollen grains deposited in the PaldDat database [3], 43% are oblate, and their proportion is higher in grain classes with a higher number of apertures. Among grains with six or more colpate/colporate apertures (positioned and elongated along the meridians of the grain), 91% are oblate. The harmomegathy of oblate pollen grains is limited by geometry. It can be shown in a simple calculation in which a pollen grain with N colpate/colporate apertures is represented by an N-gonal bicupola (Fig. 1), that there is a maximum oblateness of the pollen grain after which colpate/colporate apertures cease to be functional. This raises interesting questions regarding the exceptionally high prevalence of oblate pollen grains in grain classes and plant species with a high number of apertures.



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[2] E. Katifori, S. Alben, E. Cerda, D.R. Nelson, & J. Dumais, Foldable structures and the natural design of pollen grains, Proc. Natl. Acad. Sci. U.S.A. 107 (17) 7635-7639 (2010)
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back to the program

Developing an implicit solvation machine learning model for ionic media

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Molecular dynamics (MD) simulations of biomolecular systems require a balance between physical accuracy and computational efficiency. All-atom simulations – consisting of fully atomistic DNA, explicit water molecules, and explicit Na^+/Cl^- ions – capture detailed ion-solute interactions but become prohibitively expensive due to the large number of solvent degrees of freedom. Coarse-graining and implicit solvent models offer substantial computational savings, yet each has limitations: implicit electrostatic descriptions efficiently capture long-range interactions but lack short-range accuracy, whereas coarse-grained force fields often fail to reproduce essential many-body correlations. To overcome these limitations, we develop a Δ-learning framework in which a graph neural network (GNN) is trained on the difference between all-atom MD forces and those obtained from a computationally inexpensive implicit electrostatic prior. The model employs a coarse-grained (CG) representation of DNA, consistent across GNN training and MD simulations, while ions remain explicit and water is coarse-grained out. This enables the ML model to recover the missing short-range, many-body ion-DNA interactions, while the implicit electrostatic description provides the correct long-range behavior. Applied to CG DNA in a sodium chloride solution, the model reproduces structural observables with high fidelity relative to the all-atom MD reference, while operating at a lower computational cost.

[1] A. Coste, E. Slejko, J. Zavadlav, and M. Praprotnik, Developing an implicit solva- tion machine learning model for molecular simulations of ionic media, J. Chem. Theory Comput. 20, 411-420 (2023)

back to the program

Quantitative prediction of protein allostery

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Ligands binding to a protein can influence distant sites beyond the binding site itself – a phenomenon known as allostery, which is intrinsic to all proteins. The ability to quantitatively predict allosteric effects prior to experimental studies could significantly accelerate drug discovery and reduce associated costs. In the simple case of two ligands binding to the same protein, allosteric cooperativity can be characterized by a cooperativity parameter that quantifies how binding of one ligand affects the binding affinity of the other. From a statistical mechanics perspective, such effects emerge from a shift in the protein's conformational ensemble – the distribution of all possible structural states the protein can adopt. Specifically, each conformation (microstate) within this ensemble has a distinct probability of being realized in each of the four ligation states: unbound (free), bound to one ligand, bound to the other ligand, or bound to both. Molecular dynamics (MD) simulations enable sampling of these conformational ensembles in all four ligation states

and thus provide access to the underlying microstate probabilities. With these in hand, the cooperativity parameter can be calculated directly, allowing quantitative prediction of allosteric effects based purely on simulation data.

back to the program

On the effects of differential stress on properties of lipid bilayers

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Differential stress denotes a state of the lipid bilayer membrane in which one of its leaflets is stretched and the other one compressed. The corresponding isssues were at the mesoscopic level traditionally discussed in terms of the so called "area difference" or "non-local bending" membrane elasticities. Recently it has been suggested that sufficiently strong differential stress may affect membrane properties such as membrane bending stiffness (Hossein and Deserno, Biophys. J. 118, 624-642, 2020). The aim here is to point out that it is in this reasoning important to take into consideration typical time periods that membrane can spend in a state of differential stress. In this respect we shall shortly review a set of already historical experiments on pulling a narrow membrane tube out of an aspirated phospholipid vesicle and their theoretical interpretations. The crucial steps in this research were (i) the realization that the equilibrium relation between the tube radius and the applied pulling force corresponds to the free energy maximum, and (ii) the notion about a possible, by the non-local bending induced relaxation of this system by an advective flow of phospholipid molecules from the dense to the dilated membrane leaflets.

back to the program

Coherent modeling of double-folded ring polymers and their underlying random tree structure

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[2]ENS de Lyon, CNRS, Laboratoire de Physique (LPENSL UMR5672) et Centre Blaise Pascal, Lyon,France

Topologically constrained genome-like polymers often double-fold into tree-like configurations, which can be modeled on the level of the folded (ring) polymer or on the level of the underlying random tree. For both descriptions, we have recently obtained expressions for the configurational entropy in ensembles with controlled branching activity. In my presentation, I will demonstrate that they are equivalent up to a contribution originating from the number of distinct wrappings of a single tree and obtain an exact mapping between the two ensembles for models, where excluded volume interactions are treated consistently on the tree and on the ring level. I will also present a grand canonical version of the Amoeba Monte Carlo algorithm for simulating lattice trees with a statistical weight corresponding to the number of distinct wrappings. While the results are in excellent agreement with data from Monte Carlo simulations of the corresponding elastic lattice model for tightly double-folded rings, the new algorithm is faster. In the last part of my talk, I will show how these models are currently being used to mimic biological data.

back to the program

Detection and classification of low-complexity RNA sequences

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Biological RNA sequences can show significant statistical deviations from randomness, often presenting as subsequences with nonuniform nucleotide distribution or regions containing multiple exact or inexact repeats of a shorter motif. These regions are traditionally termed low-complexity regions (LCRs), as they can be characterized through various measures of linguistic or computational complexity. LCRs found in RNAs are increasingly recognized as functionally important, playing roles in mediating RNA-RNA interactions and driving the phase separation of long noncoding RNAs. Only a few methods currently exist for detecting the presence and location of LCRs. We present a method inspired by k-mer alignment and recurrence quantification analysis, and test it on sets of synthetically constructed RNAs with well-defined LCR positions, as well as on biological sequences known to contain functionally important LCRs. Discrepancies in detected regions underscore that no single, universal definition of an LCR can fully capture the diversity of patterns found in biological RNA.

back to the program

Liquid drops meet star polymers

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We employ the liquid drop model of deformable colloidal particles [1,2,3] so as to describe the behavior of star polymers confined between parallel plates. Using simple 2D variational ansätze, we theoretically explore the geometry of small clusters of attractive model drops and we compare the results to shapes seen in molecular-dynamics simulations of a bead-and-spring representation of the stars. We map the microscopic parameters of the bead-and-spring model on the effective parameters of the liquid drop model, thereby providing a molecular-level interpretation of the latter. In addition, the comparison unravels previously unknown features of the internal structure of confined star polymers.

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[2] A.-K. Doukas, C. N. Likos, and P. Ziherl, Structure formation in soft nanocolloids: Liquid-drop model, Soft Matter 14, 3063 (2018)
[3] F. I. Vrban, A. Šiber, and P. Ziherl, Contact Forces in Microgel Suspension, submitted

back to the program

Mechanics of cell aggregates as models of tumors and tumor spheroids

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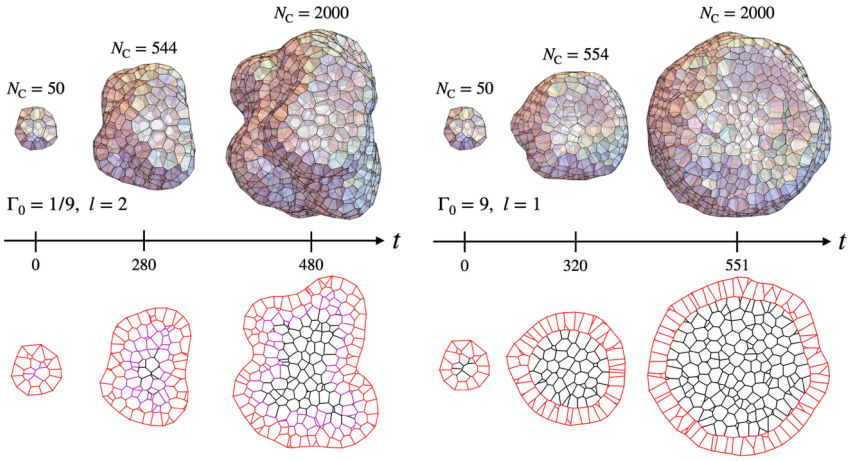
The vertex model is a reliable tool for modeling two-dimensional (2D) biological epithelial tissues, but in three-dimensional (3D) systems some of its limitations become apparent due to the computational complexity of the problems. This mainly arises from the complexity of the topological changes that occur in active tissues. The graph vertex model allows us to model 3D epithelial tissues such as tumors and tumor spheroids, where epithelial cells are represented as polyhedra. The model provides a simpler implementation of the tissue's topological transformations: cell rearrangements and cell divisions. The graph vertex model also generalizes topological transformations in two and three dimensions. Here we present tumors with free boundary conditions that grow due to cell divisions in the outer layers of the tumor. We simulate the growth of tumor spheroids by combining diffusion and consumption of nutrients with mechanical interactions. Our results show that the nutrient penetration depth and the mechanical tension between live and necrotic regions decisively influence tumor morphology: in general, shallow nutrient availability and low tension promote irregular, lobulated (finger-like) growth, whereas deeper penetration and higher tension lead to compact, spherical tumors. In addition, exponential decay of nutrients produces more irregular tumor shapes than a step-like profile. This work demonstrates that the graph vertex model is a versatile computational tool for investigating tissue morphogenesis, tumor development, and the mechanical regulation of tissue growth.



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