

Guanajuato, Mexico



*2<sup>nd</sup> International Workshop  
on Matter Out of  
Equilibrium*

BOOK OF ABSTRACTS

22-26 August 2016

# Scientific Program

	Sunday 21/8	Monday 22/8	Tuesday 23/8	Wednesday 24/8	Thursday 25/8	Friday 26/8
8:30-9:00		Opening				
9:00-10:30		Brady	McKenna	Haslam	Leheny	Castillo
		Voigtmann	Royall	Liu	Egelhaaf	Villanueva Romo
		Sevilla	Ramírez	Medina	Pine	Cortés
						Perera
10:30 - 11:00	C O F F E E    B R E A K					
11:00 - 12:00		Alarcón	P. Mendoza	Olais	Cárdenas	Sastre
		A. Torres	Lázaro	López	Arenas	
		Sanchez	Valadez	Moctezuma	L. Torres	Closing Remarks
		Vélez		B. Mendoza	Rodríguez	
12:00 - 13:00		Heinen	Conrad	Méndez	Delgado	
		Maldonado	Laurati	Castañeda	Arauz	
13:00 - 15:00		L U N C H	L U N C H	L U N C H	L U N C H	
15:00-16:00	Arrival	Báez	Donado	FREE	Elizondo	
		Castro	Sarmiento		Pérez	
Blanco		Tavera	Foffi			
Valencia		Farias				
16:00 - 16:30		C O F F E E B R E A K	C O F F E E B R E A K		C O F F E E B R E A K	
16:30 - 17:00						
17:00-20:00		Discussion	Discussion		FREE	
20:00		DINNER	DINNER		DINNER	

## **Invited Talks**

- José Luis Arauz** *From Ballistic to Diffusive Motion in Granular Matter*
- Cesar Baez** *Long-time self-diffusion for hard spheres on free-surfaces*
- John Brady** *Forces, Stresses and the (Thermo?)dynamics of Active Matter*
- Rolando Castillo** *Out-of-Equilibrium Assembly of Colloidal Particles at Air/Water Interface Tuned by Their Chemical Modification*
- Ramón Castañeda** *Effective interactions between colloids close to a thermodynamic phase transition and nearby the boundary of gelation*
- Pavel Castro** *Correctness in diffusion: The importance of curvature*
- Jacinta Conrad** *Non-equilibrium solidification in colloid-polymer mixtures with competing attractions and repulsions: dispersity effects*
- Jorge Delgado** *Some chemical and biological out-of-equilibrium systems where soft matter offers a solution to go further*
- Fernando Donado** *Glass transition, aging and aging frustration in a non-vibrating granular model for a glass forming liquid*
- Stefan Egelhaaf** *Single-particle structure and dynamics during the application of shear*
- Luis Fernando Elizondo** *General overview of glassy dynamics and dynamically arrested states in binary mixtures of hard-spheres: decoupling, mixed states and bifurcation*
- Giuseppe Foffi** *Dynamic transition and memory encoding in glass-formers under shear*
- Andrew Haslam** *Fluid-fluid coexistence in an athermal colloid-polymer mixture: thermodynamic perturbation theory and continuum MD simulation*

<b>Marco Heinen</b>	<i>Statistical mechanics for nonreciprocal effective particle interactions</i>
<b>Marco Laurati</b>	<i>Directed Percolation: an equilibrium pre-transition towards non-equilibrium arrested gel states</i>
<b>Robert Leheny</b>	<i>Coherent x-ray studies of nano-plasticity in soft glassy materials</i>
<b>Yun Liu</b>	<i>From the depletion attraction to the bridging attraction: the effect of solvent molecules on colloidal gelation transitions</i>
<b>Amir Maldonado</b>	<i>Foams made with surfactant bilayer phases</i>
<b>Gregory McKenna</b>	<i>Open Questions in Glassy Physics: Is there an ideal glass transition and are colloidal dispersions good models of glasses?</i>
<b>Magdaleno Medina</b>	<i>Non-Equilibrium Statistical Thermodynamics: A Tool for Describing Amorphous Solidification</i>
<b>José Méndez</b>	<i>Single-file diffusion on a circle: Temporal regimes and scaling laws</i>
<b>David Pine</b>	<i>Random Organization: Critical dynamics and hyperuniformity in periodically sheared suspensions</i>
<b>Pedro Ramírez</b>	<i>Towards the construction of a fundamental statistical theory of non-equilibrium and arrested systems</i>
<b>Patrick Royall</b>	<i>Non-equilibrium phase transition to an ideal glass?</i>
<b>Erick Sarmiento</b>	<i>Anisotropic colloids in laser-induced external potentials: an energy landscape approach</i>
<b>Francisco Sastre</b>	<i>TBA</i>
<b>Francisco Sevilla</b>	<i>Transport equations for active swimmers</i>
<b>Nestor Valadez</b>	<i>Structure of colloidal gels at intermediate concentrations: the role of competing interactions</i>

**Thomas Voigtmann**

*Slow Dynamics of Self-Propelled Particles*

## **Contributed Talks**

**Francisco Alarcon**

*Phase behaviour of attractive microswimmers*

**Brisa Arenas**

*Dynamics of shear banding flow in Non-Newtonian fluids*

**Rodolfo Blanco**

*Stress distribution in two-dimensional silos*

**Heliana Cardenas**

*Sedimentation of Particles in Viscoelastic Fluids*

**Ernesto Cortés**

*Equilibration and Aging of Liquids of Non-Spherically Interacting Particles*

**Mariana Farias**

*Thermodynamic properties of 1:1 electrolyte solutions in the Statistical Associating Fluid Theory plus Binding in the Mean Spherical Approximation Theory*

**Edilio Lazaro**

*Equilibrium and non-equilibrium states in binary mixtures*

**Leticia Lopez**

*Linear viscoelasticity on arrested spinodal decomposition*

**Birzabith Mendoza**

*Modified collagen gel networks: preparation and biomedical applications*

**Patricia Mendoza**

*The discontinuous ideal glass transition, a soft crossover at finite waiting times*

**Rosario Moctezuma**

*Complexity of a system of non-vibrational steel beads under a time-dependent magnetic field*

**Adriana Nicasio**

*Counterion accumulation effects on a suspension of DNA molecules: equation of state, effective charge and denaturation profile*

**Manuel Olaís**

*Formation of amorphous solids by arrested spinodal decomposition*

<b>Jorge Perera</b>	<i>Assessment of the micro-structure and depletion potentials in two-dimensional binary mixtures of additive hard-disks</i>
<b>Sarai Romo</b>	<i>Interactions between Liposomes and Nitrogen-Doped Carbon Nanotubes: new composites for possible applications</i>
<b>Gustavo Rodriguez</b>	<i>Long-range effective potential between granular rods within a granular medium</i>
<b>Manuel Sanchez</b>	<i>Visualization of membrane of E. Coli using deconvolution in brightfield and fluorescence</i>
<b>Antonio Tavera</b>	<i>Light absorbing scattering techniques in soft matter</i>
<b>Alexis Torres</b>	<i>Transport properties of a single nano-colloid from molecular dynamics</i>
<b>Luis Torres</b>	<i>Runout transition in bidimensional dumbbell-like rock avalanches</i>
<b>Dulce Valencia</b>	<i>Semiflexible physical curves under confinement or affected by environmental conditions</i>
<b>Rodrigo Velez</b>	<i>On the motion of carbon nanotube clusters near optical fiber tips: effects of thermal convection and thermophoresis</i>
<b>José Ramón Villanueva</b>	<i>Short-time dynamics of monomers and dimers in quasi-two-dimensional colloidal mixtures</i>

**Abstracts:**

**Invited Talks**

## Forces, Stresses and the (Thermo?)dynamics of Active Matter

John F. Brady\*<sup>a</sup>, Sho Takatori<sup>a</sup>, and Wen Yan<sup>a</sup>

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A core feature of many living systems is their ability to move, to self-propel, to be active. Through their motion, either voluntarily or involuntarily, living systems are able to self-assemble or swarm. But such behavior is not limited to living systems. Recent advances in colloid chemistry have led to the development of synthetic nonliving particles that are able to undergo autonomous motion by converting chemical energy into mechanical motion and work – chemical swimming. Through their self-motion, “active matter” systems generate their own internal stress, which can drive them far from equilibrium and free them from conventional thermodynamic constraints, and by so doing active matter can control and direct its own behavior and that of its surroundings [refs. 1-4]. In this talk we examine the unique mechanical “swim pressure” exerted by all active systems and demonstrate how activity imparts new behaviors to active matter that distinguish it from equilibrium condensed matter systems.

[1] S.C. Takatori, W. Yan and J.F. Brady, *Phys. Rev. Lett.*, **113**, 028103 (2014).

[2] S.C. Takatori and J.F. Brady, *Phys. Rev. E*, **91**, 032117 (2015).

[3] S.C. Takatori and J.F. Brady, *Current Opinion in Colloid & Interface Science*, **21**, 24 (2016).

[4] S.C. Takatori, R. De Dier, J. Vermant, J.F. Brady, *Nature Commun.*, **7**:10694 (2016).



## Slow Dynamics of Self-Propelled Particles

Thomas Voigtmann\*<sup>a,b</sup>, Alexander Liluashvili<sup>a</sup>

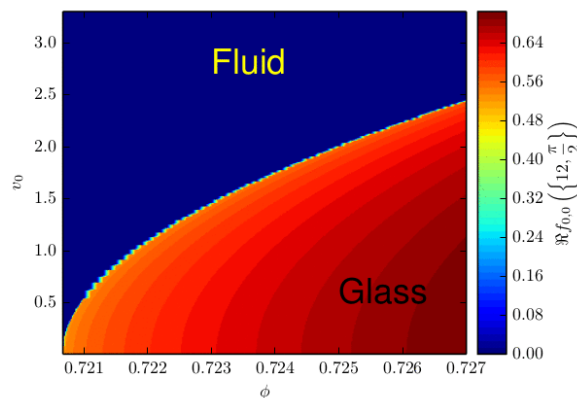
<sup>a</sup> *Institute of Materials Physics in Space, German Aerospace Center (DLR), Köln, Germany*

<sup>b</sup> *Heinrich-Heine-Universität Düsseldorf, Germany*

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Self-propelled Brownian particles are model systems for microswimmers such as bacteria or driven suspensions of colloidal Janus particles. The motion of self-propelled particles through crowded environments reveals an interplay between slow dynamics caused by obstacles or the excluded volume interactions among the particles, and the nonequilibrium driving mechanism.

In this talk, I discuss in particular the glassy dynamics in a system of dense active Brownian particles whose activity is characterized by a self-propulsion speed and the rotational diffusion mimicking persistent motion. Based on a recent extension of mode coupling theory for this system, the glass transition is found to shift with the self propulsion, and the dependence of the dynamics on the orientational Peclet number. Time permitting, I will also briefly discuss the critical dynamics of a food-consuming particle in a porous medium.



**Figure 1:** Glass-transition diagram of active Brownian particles as a function of two-dimensional packing fraction and self-propulsion velocity.

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**Transport equations for active swimmers**

Francisco J Sevilla<sup>\*a</sup>, Juan Manuel Pérez Peña <sup>a</sup>

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During the last two decades a fast-growing interest on the statistical mechanics of active motion has taken place. Active motion, which is the result of the transformation of energy taken from the environment and transformed into motion, is observed in a variety of biological organisms and in a diversity of man-made particles. The mechanisms of energy conversion can be very complex, and different mathematical frameworks to describe particular patterns of active motion have been devised, being active Brownian motion and Run-and-tumble, the ones more recurrently considered. In this contribution we argue that the transport equation is a suitable framework for the description of a variety of patterns of motion of active swimmers, including active Brownian motion and run-and-tumble particles. We present analytical expressions for the two-dimensional probability density  $P(\mathbf{x},t)$ , of finding a particle at position  $\mathbf{x}$  at time  $t$ , independent of its direction of motion, solution of the transport equation. Effects of chirality on the patterns of motion are naturally included in the formalism developed.

We acknowledge financial support from Programa UNAM-DGAPA-PAPIIT IN113114.

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**Statistical mechanics for nonreciprocal effective particle interactions**

M. Heinen<sup>\*a</sup>, J. Bartnick<sup>b</sup>, C.-R. Du<sup>c</sup>, V. Nosenko<sup>d</sup>, Hartmut Löwen<sup>b</sup>, A.V. Ivlev<sup>e</sup>

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We present our theoretical, experimental and computer simulation studies of two different types of soft matter systems. Both systems exhibit nonreciprocal effective particle interactions that break Newton's third law on coarse-grained length- and time-scales. The first type of system is a complex (dusty) plasma, where two species of micron-sized particles levitate in parallel bilayers above an electrode [1]. In the non-equilibrium environment of a dilute flowing plasma, the particles experience nonreciprocal effective electrostatic interactions which result in a temperature splitting that is predicted by kinetic theory, and observed in Molecular Dynamics simulations as well as experiments: In a non-equilibrium steady state, each of the two particle species acquires a separate temperature, such that the average kinetic energy gain in an inelastic collision vanishes. The second system is a Brownian suspension of bidisperse, mutually diffusiophoretic particles [2]. Here, every particle is a source of a chemoattractant (or repellent) substance, and the particles undergo diffusiophoretic motion in the resulting density profiles of the chemical substances. Nonreciprocal effective interactions are observed in cases where the diffusiophoretic mobilities or the chemical substance release rates are unequal for both particle species, or when the chemical substances exhibit different diffusion coefficients or evaporation rates. As a consequence of action-reaction symmetry breaking in the Brownian suspension, we observe peculiar particle pair correlations in Brownian Dynamics simulations, which are in good agreement with our numerical solution of the many-body generalized Smoluchowski equation.

[1] A.V. Ivlev, J. Bartnick, M. Heinen, C.-R. Du, V. Nosenko, H. Löwen, PRX 5, 011035 (2015).

[2] J. Bartnick, M. Heinen, A.V. Ivlev, H. Löwen, JPCM 28, 025102 (2016).

**Foams made with surfactant bilayer phases**

Amir Maldonado

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Liquid foams are dispersions of gas bubbles in a liquid, stabilized by surface active molecules like surfactants. They are unstable systems that age and eventually disappear due to different mechanisms: drainage, coalescence and coarsening. Most foaming solutions contain surfactant molecules in the micellar phase. Recently, it has been of interest to study foams made with other surfactant phases, like those composed of bilayers. In this talk we describe experiments performed to assess the stability of foams made with sponge and lamellar bilayer phases. The results show that the lamellar phase produces very stable foams due to its high viscosity which slows down drainage. On the contrary, the foams made with sponge phases are very unstable probably due to a facilitated coalescence due to the disordered local structure.

## Long-time self-diffusion for hard spheres on free-surfaces

César Alejandro Báez<sup>a\*</sup>, J. Alejandro Ortega-Gutiérrez<sup>a</sup>, José M. Méndez-Alcaraz<sup>b</sup>,  
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In order to calculate the dynamical properties of hard systems; a recently proposed continuous pseudo hard sphere potential[1] for molecular dynamics is studied in the context of hard spheres deposited on free-surfaces by means of Brownian dynamics simulations (BD). Although the long-time self-diffusion coefficient  $D_s^L$  from this simulations agree well with the experimental data[2,3], there exists fluctuations from the experiments around the  $D_s^L$  obtained from simulations. To study the origin of this fluctuations, we use the Smoluchowski equations and the full two-body HI theory to show that the effects of HI in the the second moment for the self-intermediate scattering function are strongly correlated with the fluctuations that the experimental  $D_s^L$  shows around the one calculated from BD and dynamic Monte Carlo simulations without HI.

[1] J. Jover, *et al.*, *J. Chem. Phys.* **137**, 144505 (2012).

[2] A. L. Thorneywork *et al.*, *J. Chem. Phys.* **140**, 161106 (2014).

[3] A. L. Thorneywork *et al.*, *Phys. Rev. Lett.* **145**, 268301 (2015).

## Correctness in diffusion: The importance of curvature

Pavel Castro Villarreal\*<sup>a</sup>

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Diffusive processes on curved manifolds have gained increased attention over the last decades. The lateral diffusion transport phenomenon of integral membrane proteins or lipids in a biological cell is a related and interesting complex process, mainly due to the interaction with the remaining components of the membrane, the protein-size effects and the shape undulations produced by thermal fluctuations; all these contributions have allowed for complementary points of view to approach the problem (see [1,2] and references within). In this occasion, inspired by the Saffman-Delbrück seminal contribution, we study the role of geometry in the transport processes occurring within the membrane. In particular we establish a general dependence between the transport phenomena and the membrane's geometry.

- [1] Pavel Castro-Villarreal, *J. Stat. Mech.*, **P08006** (2010); Pavel Castro-Villarreal, *J. Stat. Mech.*, **P05017** (2014);
- [2] Pavel Castro-Villarreal, Alejandro Villada-Balbuena, José Miguel Méndez-Alcaraz, Ramón Castañeda-Priego, and Sendic Estrada Jiménez, *J. Chem. Phys.* **140**, 214115 (2014)

**Open Questions in Glassy Physics: Is there an ideal glass transition  
and are colloidal dispersions good models of glasses?**

Gregory B. McKenna<sup>a</sup>

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The glass transition event is frequently taken to be a manifestation of an underlying thermodynamic transition, perhaps 50 K below the laboratory measured glass transition temperature. The behavior of glasses manifests itself in both the thermodynamic and dynamic responses and these are frequently interpreted in terms of an ‘ideal’ glass transition. Here we first examine the thermodynamics by using calorimetric measurements to determine the equilibrium heat capacity of a series of poly( $\alpha$ -methyl styrene) mixtures with results that show no evidence of a transition in the Ehrenfest sense as far as 150 K below the nominal glass transition temperature[1]. The dynamic signature of glasses is found in the super-Arrhenius behavior of viscosity or relaxation time as a function of temperature. The so-called Vogel-Fulcher extrapolation of the measured dynamic property leads to an apparent finite-temperature divergence some 50 K below the nominal glass temperature. By performing experiments on glasses aged for very long times (Dominican amber of 20 million years) we[2] have been able to explore the upper bounds to the equilibrium dynamics to some 43.6 K below the glass temperature and find strong evidence that the finite-temperature divergence does not exist, rather the glass exhibits an apparent Arrhenius behavior for the dynamics, suggesting that theories that are based on the finite temperature divergence of the relaxation times need to be re-evaluated. Finally, there is considerable activity in the Soft Matter community in which concentrated colloidal dispersions are used as models of glass-forming systems. Here we visit this problem using a novel series of concentration-jump experiments in PNIPAAm-particle colloids to mimic the classic temperature-jump experiments that were used by Kovacs to catalogue the kinetics of structural recovery in molecular glasses. Here we will use diffusing wave light scattering spectroscopy and classical rheological methods to examine specifically the “intrinsic” isotherm, asymmetry of approach, and the memory signatures and compare the colloidal system with the molecular glass. We find that the colloidal systems while exhibiting some of the features seen in molecular glasses, in detail show surprising differences in their structural recovery signatures[3].

[1] D. Huang, S.L. Simon and G.B. McKenna, "Equilibrium Heat Capacity of the Glass-Forming Poly( $\alpha$ -methyl styrene) Far below the Kauzmann Temperature: The Case of the Missing Glass Transition," *J. Chem. Phys.*, **119**, 3590-3593 (2003).

[2] J. Zhao, S.L. Simon, G. B. McKenna, "Using 20-million-year-old amber to test the super-Arrhenius behavior of glass-forming systems," *Nature Comm.*, **4**, 1783-1 - 1783-6 (2013).

[3] X. Peng and G.B. McKenna, "Physical Aging and Structural Recovery in a Colloidal Glass Subjected to Volume Fraction-Jump Conditions," *Physical Review E.*, **93**, 042603 (2016).

## Non-equilibrium phase transition to an ideal glass?

C. Patrick Royall<sup>abcd</sup>, Rattachai Pinchaipat<sup>ac</sup>, Matteo Campo<sup>c</sup>, James Hallett<sup>ac</sup>,  
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The glass transition is one of the longstanding challenges in condensed matter. In particular, one seeks to understand how solidity emerges with little apparent change in structure [1]. A central aspect for the understanding of supercooled liquids is dynamic heterogeneity: on suitable observation time scales, local regions appear liquid-like (*active*) or solid-like (*inactive*), suggesting that any successful explanation must naturally include this phenomenon. A variety of theories have been proposed, indeed whether the glass transition has a thermodynamic (implying structural) or dynamical origin remains unclear. The former may be related to a transition to an ideal glass state at finite temperature with minimal configurational entropy[1,2].

Among the key developments supporting the dynamical picture is the discovery of a non-equilibrium phase transition in trajectory space which reveals phase coexistence between the normal supercooled liquid (active phase) and a glassy state (inactive phase) [1]. Until now, such non-equilibrium transitions have been limited to numerical and theoretical studies [2], but here we present evidence that such a transition occurs in experiment. We identify trajectories in a model glassformer, colloidal hard spheres, using particle-resolved studies. Our analysis reveals a non-Gaussian distribution of trajectories leaning towards those rich in locally favoured structures (LFS)], which are associated with the emergence of slow dynamics in the hard sphere system we study [3-6]. This we interpret as evidence for a non-equilibrium transition to an inactive LFS-rich glass similar to an ideal glass, which we confirm by reweighting trajectory data. We discuss how our results may be used to unify the disparate theoretical approaches to the glass transition.

[1] C.P. Royall and S.R. Williams, *Phys. Rep.* **560** 1-75 (2015).

[2] T. Speck, A. Malins, and C. P. Royall, *Phys. Rev. Lett.* **109**, 195703 (2012).

[3] F. Turci, C. P. Royall and T. Speck, *arXiv:1603.06892* (2016).

[4] C. P. Royall, A. Malins, A. J. Dunleavy, and R. Pinney, *J. Non-Cryst. Solids* **407**, 34 (2014).

[5] A.J. Dunleavy, K. Wiesner, R. Yamamoto, and C.P. Royall, *Nature Communications*, **6** 6089 (2015).

[6] R.L. Jack, A.J. Dunleavy, and C.P. Royall, *Phys. Rev. Lett.*, **113** 095703 (2014).



**Towards the construction of a fundamental statistical theory of non-equilibrium and arrested systems**

Pedro E. Ramírez-González<sup>\*a</sup>, Luis E. Sanchez-Díaz<sup>b</sup>, Magdalena Medina-Noyola<sup>c</sup>

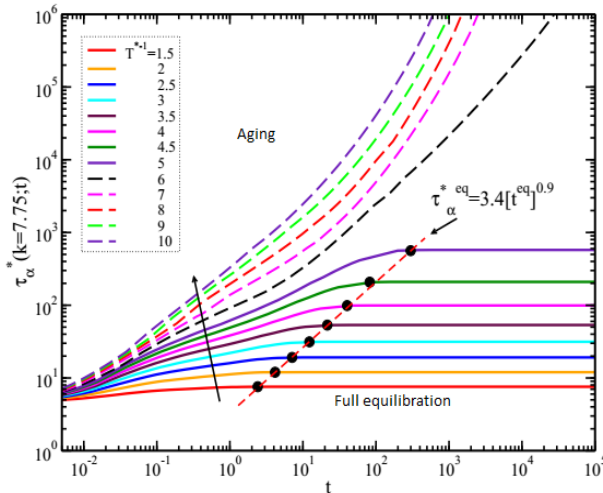
<sup>a</sup> CONACYT - Instituto de Física "Manuel Sandoval Vallarta", Universidad Autónoma de San Luis Potosí, Álvaro Obregón 64, 78000 San Luis Potosí, SLP, México.

<sup>b</sup> Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA.

<sup>c</sup> Instituto de Física "Manuel Sandoval Vallarta", Universidad Autónoma de San Luis Potosí, Álvaro Obregón 64, 78000 San Luis Potosí, SLP, México.

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A non-equilibrium extension of Onsager's canonical theory of thermal fluctuations is employed to derive a self-consistent theory for the description of the statistical properties of the instantaneous local concentration profile of a colloidal liquid in terms of the coupled time evolution equations of its mean value and of the covariance of its fluctuations [1]. These two coarse grained equations involve a local mobility function which, in its turn, is written in terms of the memory function of the two-time correlation function. This theory, known as the Non-Equilibrium Self-Consistent Generalized Langevin Equation (NE-SCGLE) theory, also provides a general theoretical framework to describe irreversible processes associated with dynamic arrest transitions, such as aging, and the kinetics of glass and gel formation [2,3]. In addition, selected applications are introduced in order to illustrate the predictive power of the theoretical framework.



**Figure 1:** For a simpler model colloidal liquid involving only soft repulsive interactions that follows a sudden temperature quench, the NE-SCGLE theory predicts two types of behavior; full equilibration and aging, which are illustrated in the figure. We plot the  $\alpha$ -relaxation time for a sequence of quench processes at fixed volume fraction, from fixed initial temperature  $T_0$  to a different values of the final temperature  $T_f$  both above and below the dynamic arrest temperature  $T_c$ . The theory also define an equilibration time  $t^{eq}(T)$ , as the time after which  $\tau_\alpha(t)$  has attained its equilibrium value  $\tau_\alpha^{eq}(T)$ . It is predicted that both,  $t^{eq}(T)$  and  $\tau_\alpha^{eq}(T)$ , diverge as  $T$  approaches  $T_c$  from above, and remains infinite for  $T < T_c$ . The fill circles highlight the points  $(t_{eq}^*(T^*), \tau_{eq}^*(T^*))$  which obey the approximate relation  $\tau_{eq}^*(T^*) \approx 3.4 \times [t_{eq}^*(T^*)]^{0.9}$ . This scenario is enriched when the systems involves attractive interactions and other arrested states appears such as gels.

- [1] P. Ramírez-González and M. Medina-Noyola, *Phys. Rev. E* **82**, 061503 (2010).  
 [2] L. E. Sánchez-Díaz, P. Ramírez-González and M. Medina-Noyola, *Phys. Rev. E* **87**, 052306 (2013).  
 [3] J. M. Olais-Govea, L. López-Flores and M. Medina-Noyola, *J. Chem. Phys. E* **143**, 174505 (2015).

## Structure of colloidal gels at intermediate concentrations: the role of competing interactions

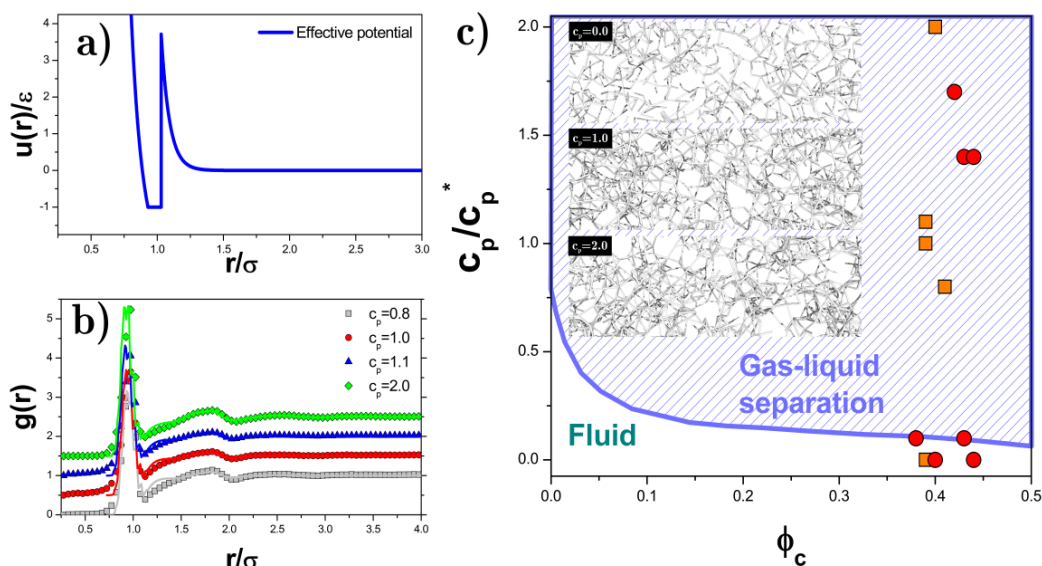
Néstor E. Valadez-Pérez<sup>\*a</sup>, Ronja F. Capellmann<sup>b</sup>, Benedikt Simon<sup>b</sup>, Stefan U. Egelhaaf<sup>b</sup>, Marco Laurati<sup>a</sup> and Ramón Castañeda-Priego<sup>a</sup>

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In this work we demonstrate that the effective particle interaction in an intermediate volume fraction colloidal gel can be accurately described in terms of competing interactions. The latter include a short-range attractive contribution due to the addition of non-adsorbing polymers and a long-range repulsive part associated to the presence of residual charges on the colloid surface. We analyze particle positions, obtained through confocal microscopy, and performed Monte Carlo simulations. The comparison between the radial distribution function obtained from the experiment and simulation let us to adjust the interparticle potential that best reproduces the experimental structure (see Fig. 1 a) and b)). In addition, we briefly revisit the state diagram of a colloid-polymer mixture, pointing out the relevance of the competing interaction on determining the local structure of a gel (see Fig. 1 c)).



**Figure 1:** a) Effective pair potential for colloidal particles in a suspension with added polymer. b) Radial distribution function obtained from the experiment (symbols) and from Monte Carlo simulation in samples with different polymer concentration. c) Phase diagram for the colloid-polymer mixture, symbols correspond to the samples we analyzed. The snapshots show the local structure of the colloidal system for samples with different polymer concentration, every cylinder indicates the bond between two particles.

## Non-equilibrium solidification in colloid-polymer mixtures with competing attractions and repulsions: dispersity effects

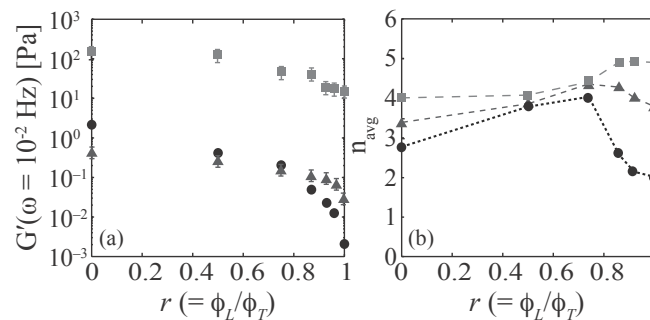
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Submicron particles suspended in complex fluids containing surfactants, polymers, micelles, or other species are widely used in materials shaping and forming processes, including three-dimensional printing and nanocomposite processing, and in technical applications as paints, coatings, inks, and drilling muds. These applications require control over suspension rheology and microstructure, which are affected by interactions between the different constituents. Practically, constituents of high dispersity in size or molecular weight are inexpensive and hence widely used; fundamentally, the effects of size dispersity on suspension properties remain poorly understood, especially when the particles exhibit attractive as well as repulsive interparticle interactions. As simple models of practical suspensions we formulate mixtures of submicron poly(methyl methacrylate) particles suspended in solutions of non-adsorbing polystyrene polymers, which generate a controlled entropic depletion attraction between the particles. Here, I will discuss studies in which we investigate the effect of particle dispersity and polymer dispersity on the non-equilibrium phase behaviour, microstructure, and rheology of these colloid-polymer mixtures.



**Figure 1: Summary of metrics for mechanical and structural changes with particle size dispersity ratio for mixtures of polymers and bidisperse colloids. (a) Elastic modulus at a frequency of  $10^{-2}$  Hz,  $G'(\omega = 10^{-2} \text{ Hz})$  and (b) average bond number  $n_{\text{avg}}$  as a function of volume fraction of large particles  $r$  for all three series of experiments: Series 1 (particle volume fraction  $\phi = 0.15$  and particle size ratio  $\alpha = a_s/a_L = 0.31$ , circles), Series 2 ( $\phi = 0.15$  and  $\alpha = 0.45$ , triangles), and Series 3 ( $\phi = 0.40$  and  $\alpha = 0.31$ , squares). Adapted from ref [1].**

**Directed percolation: an equilibrium pre-transition towards non-equilibrium arrested gel states**

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The macroscopic properties of gels arise from their slow dynamics and load bearing network structure, which are exploited by nature and in numerous industrial products. However, a link between these structural and dynamical properties has remained elusive. In this talk I will present confocal microscopy experiments and simulations of gel-forming colloid-polymer mixtures. They reveal that gel formation is preceded by continuous and directed percolation. Both transitions lead to system spanning networks, but only directed percolation results in extremely slow dynamics, ageing and a shrinking of the gel that resembles syneresis. Therefore, dynamical arrest in gels is found to be linked to a structural transition, namely directed percolation, which is quantitatively associated with the mean number of bonded neighbours. Directed percolation denotes a universality class of transitions. Our study hence connects gel formation to a well-developed theoretical framework which now can be exploited to achieve a detailed understanding of arrested gels.

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**Glass transition, aging and aging frustration in a non-vibrating  
granular model for a glass forming liquid**

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We study experimentally a model of a glass forming liquid based on a non-vibrating magnetic granular system under an unsteady magnetic field. A sudden quenching is produced which drives the system from a liquid state to a different final state with lower temperature, the latter could be a fluid state or an arrested state. We determined the mean squared displacement in temporal windows to determine the dynamical evolution of the system. We also obtained the radial distribution function and determined its structural characteristics. The results were analyzed using the intermediate scattering function and the effective interaction potential between two particles. We observed that when the quenching drives the system to a final state in the fluid phase, equilibration occurs very quickly, however as the temperature goes closer to the glass transition temperature, the equilibration is slower. We also observed that when the final state was very inside in the arrested state region, the system reached its equilibrium state very fast. When the final state had an intermediate temperature below the corresponding glass transition temperature, the system fell into a state that evolved slowly, presenting aging. The system evolved by an aging process toward more ordered states. However after a waiting time the dynamical behavior changed qualitatively. It was observed that some particles overcome the repulsive interactions and fell into the attractive well forming small stable aggregates. The effective potential curves clearly show the emergence of a second effective well due to the attraction, which quickly evolves and results in a deeper well than the initial effective well due to the repulsion. As time went by, more particles fell into this condition. The appearing of inhomogeneities produces a frustration of the aging process.

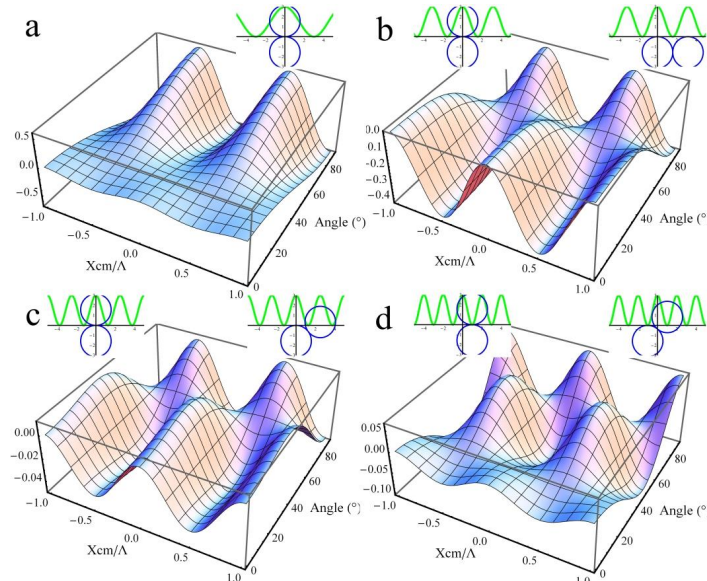
## Anisotropic colloids in laser-induced external potentials: an energy landscape approach

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In this work, the effect of a laser-induced periodical external potential on the spatial arrangement of anisotropic particles is studied both theoretically and experimentally. Periodical distribution of light is created by the interference of two coherent laser beams [1]. Using a new algorithm, based on Mie approximation for optical trapping [2], the energetic landscape of colloidal particles in a periodic distribution of light is calculated at different periodicities of the external potential. Preferred spatial configuration of the anisotropic particles, i.e. minimum energy points in the energy landscape, were found and compared with experiments for a spherical particle, a dumbbell symmetric particle and a dumbbell asymmetric particle. With this information, arrangement of higher-order clusters is straightforward and an example us such analysis is also given for a trimer colloid. Altogether, this methodology gives a new and very powerful approach for the analysis of the effect of external optical potentials on isotropic and anisotropic colloidal particles either for equilibrium or non-equilibrium dynamics [3].



**Figure 1. Energy landscape for a dumbbell particle at different periodicities:  $\Lambda/D=1.9, 1.0, 0.79, 0.63$  for a) b) c) and d) respectively; where  $\Lambda$  is the periodicity of the potential and  $D$  is the diameter of a monomer particle. In all cases insets shows a schematic representation of the stable points found.**

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**Fluid–fluid coexistence in an athermal colloid–polymer mixture:  
thermodynamic perturbation theory and continuum molecular-  
dynamics simulation**

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Using both Wertheim's thermodynamic perturbation theory (TPT1) [1,2] and continuum molecular-dynamics simulation, we examine a mixture of hard-sphere (HS) polymer chains of degree 100, and colloids, represented by HSs of diameter 20 times that of the monomer segments comprising the polymer chains. According to TPT1 this athermal system phase separates into colloid-rich and polymer-rich fluid phases. Using a continuous pseudo-HS potential developed in previous work [3], molecular-dynamics simulations are performed at a phase point indicated by TPT1 to be well within the two-phase region, from starting configurations corresponding to completely pre-mixed and completely phase-separated colloids and polymers. Clear evidence is seen of the stabilization of both simulations into two co-existing fluid phases. The peaks in the probability distributions of the densities correspond to the densities calculated using TPT1; interestingly, an analysis of the interfacial tension of the phase-separated regions indicates ultra-low tensions in line with previous values determined with square-gradient theory [4] and experiment [5] for colloid–polymer systems. Further simulations are carried out to examine the nature of these co-existing phases. Reminiscent of the Asakura-Oosawa model [6], the polymer chains are seen to be fully penetrable by other polymers however, from the point of view of the colloids, they behave (on average) as almost-impenetrable spheres. As expected, the averaged interaction between polymer molecules in the polymer-rich phase is found to be of soft-repulsive character. On the other hand, the corresponding interaction in the colloid-rich phase is revealed to be of an entirely different form, characterized by a region of effective intermolecular attraction.

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**From the depletion attraction to the bridging attraction: the effect of  
solvent molecules on colloidal gelation transitions**

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Spherical colloidal systems with depletion attractions have been widely used as model colloidal systems to study gelation and glass transitions. A depletion attraction system can be considered as a binary colloidal system with a large size asymmetric ratio, where there is no attraction between the added small solvent particles and large solute particles. However, there are a wide range of colloidal systems in which the attraction between solvent and solute particles is not negligible. The extension of the results from a depletion attraction system to other binary colloidal systems has not yet been carefully examined. In the extreme case where there is a strong attraction between solvent and solute particles, a solvent particle can serve as a bridge connecting neighboring solute particles. This kind of effective attraction between large solute particles is termed as the bridging attraction. Interestingly, it is found that there is a non-monotonic behavior of the effective bridging attraction as a function of small particle concentration[1]. Adding small particle first increases the effective attraction strength between large solute particles. However, once reaching a maximum value, further adding small particles decreases the attraction strength. This interesting concentration dependence of the bridging attraction strength results in interesting phase diagrams of bridging attraction systems. In a system consisting of large polystyrene particles and small particles synthesized with poly (N-isopropylacrylamide), we observed a liquid-gel-liquid transition experimentally by increasing the small particle concentration[2]. The similarity and difference between a depletion attraction and our bridging attraction system will be also discussed[2,3].

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## Non-Equilibrium Statistical Thermodynamics: A Tool for Describing Amorphous Solidification

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Statistical thermodynamics provides a fundamental tool to predict and understand the thermodynamic properties of matter given the microscopic forces between the constituent molecules. In spite of its beauty and universal validity, statistical thermodynamics has severe limitations when we need to describe systems and conditions in which thermodynamic equilibrium is not guaranteed. In fact, this is the case with most materials that surround the portion of the universe with which human beings interact in everyday life. For example, the properties of many structurally amorphous solids around us exhibit obvious signatures of non-equilibrium behaviour, such as a manifest dependence on preparation protocol or on the time of their measurement. This calls for the development of an extended version of statistical thermodynamics that integrates dynamic and kinetic processes and incorporates the evolution time as an explicit variable. In this talk I review the Non-equilibrium self-consistent generalized Langevin equation (NE-SCGLE) theory, which provides a theoretical description of the non-equilibrium evolution of the structural and dynamical properties of liquids during their amorphous solidification. I will briefly summarize its fundamental basis (a non-equilibrium extension with microscopic resolution of Onsager's theory of irreversible processes), its most notable achievements, and the perspectives of its further development and application.

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## Single-file diffusion on a circle: Temporal regimes and scaling laws

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We report on the diffusion of  $N$  paramagnetic colloidal particles moving on a circle of radius  $R$ . We focus on the temporal regimes obtained from Brownian dynamics simulations in curved manifolds [1]. Our findings show that the mean-square angular displacement,  $\langle[\Delta\phi(t)]^2\rangle$ , displays four temporal regimes as the time,  $t$ , passes: free diffusion ( $\sim D_0 t$ ), single-file diffusion ( $\sim\sqrt{t}$ ), cluster-like diffusion ( $\sim D_0 t/N$ ) and localization-like diffusion ( $=\pi^2/3$ ), where  $D_0$  is the Stokes-Einstein diffusion coefficient. We furthermore demonstrate that the crossover times between these regimes follow scaling laws in terms of the system parameters. This allows us to highlight that the dynamics of small and closed systems exhibits a richer behaviour than the standard scenario of single-file diffusion along a straight and infinite line, where the mean-square displacement only displays the first two regimes.

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2<sup>nd</sup> International Workshop on Matter Out of Equilibrium,  
22-26 August 2016, Guanajuato, México

**Effective interactions between colloids close to a thermodynamic  
phase transition and nearby the boundary of gelation**

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Effective interactions between colloidal particles are typically measured or calculated under equilibrium conditions and when the host medium is far away from any kind of thermodynamic transition. However, recently, it has been pointed out the importance of the thermodynamic state on the effective potential between colloids, for instance, the so-called critical Casimir forces, which emerge when the solvent experiences a gas-liquid phase separation. In this contribution, we present a theoretical framework, based on the integral equations theory for simple liquids, that is able to account for the effective forces among colloids even under situations where the system is close to a thermodynamic instability or near to the boundary of gelation. We particularly discuss a few examples, namely, binary mixtures of hard-spheres close to the so-called demixing transition and colloids immersed in a dispersion of soft particles that experience either a fluid-solid transition or a gel transition.

## Coherent x-ray studies of nano-plasticity in soft glassy materials

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Any solid under applied stress possesses an elastic limit above which it fails. Failure of ductile solids is characterized by yielding, which involves irreversible changes to the material's microstructure. In the case of amorphous solids, such as glasses, pastes, and gels, the intrinsic disorder of the materials makes identifying these changes difficult. This talk will describe x-ray photon correlation spectroscopy experiments on a set of disordered soft solids including concentrated nanocolloidal gels, clay suspensions, and nanoemulsions subjected to *in situ* oscillatory shear strain that provide unique information about the spatial character of rearrangements above yielding at the nanometer scale. The oscillatory strain causes periodic echoes in the x-ray speckle pattern, creating peaks in the intensity autocorrelation function. The peak amplitudes are attenuated above a threshold strain, signalling the onset of irreversible particle rearrangements. The gels and nanoemulsions display strain softening well below the threshold, indicating a range of strains at which deformations are nonlinear but reversible. In the gels, the wave-vector dependence of the decay rate further reveals a power-law distribution in the size of rearranging regions, suggesting a non-equilibrium critical transition at yielding.

## Single-particle structure and dynamics during the application of shear

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Concentrated colloidal liquids and dynamically arrested states, i.e. glasses, are subjected to time-dependent shear, either a step change in shear rate or shear stress. The macroscopic rheological response as well as the microscopic structure and dynamics on a single-particle level are followed using combined rheology and confocal microscopy.

Upon a step change in shear rate, the transition from a solid-like response to flow is characterized by a stress overshoot [1]. This response is linked to structural features, like cage compression, as well as transient dynamics, namely superdiffusion, which lead to cage deformation, rearrangement and, eventually, breaking [2]. Cage distortions beyond the limit given by Brownian relaxation, provide a mechanism for energy storage [3]. Even in the steady state, intermediate super diffusion is observed at high rates and is a signature of the continuous shear-induced breaking and reformation of cages.

The macroscopic creep response is quantitatively linked to the microscopic single-particle dynamics, in particular the mean squared displacement and the fraction of active regions [4]. We observe dynamical heterogeneities, namely regions of enhanced mobility, which remain localized in the creep regime, but grow for applied stresses leading to steady flow.

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2<sup>nd</sup> International Workshop on Matter Out of Equilibrium,  
22-26 August 2016, Guanajuato, México

**Random Organization: Critical dynamics and hyperuniformity in  
periodically sheared suspensions**

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Suspensions of neutrally buoyant non-Brownian particles driven by slow periodic shear can undergo a dynamical phase transition between a fluctuating irreversible steady state and an absorbing reversible state. Experiments show that there are diverging time and length scales near the phase transition, and that these can be understood in terms of a simple computer model.

## Some chemical and biological out-of-equilibrium systems where soft matter offers a solution to go further

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Matter out-of-equilibrium dominates the state of the art in many fields and represent an opportunity to interact beyond classic schemes in physics. Soft matter also offers a robust scheme to do so. In this talk, I present several out-of-equilibrium systems who recently have attracted my attention: A polymerization front of acrylic acid is basically a wave front where polymerization occurs. I show the control of this front using micelles of SDS in an ionic liquid. That control opens the possibility to gain homogeneity in density and molecular weight of the polymer. Besides polymers, chocolate is complex mixture based on cocoa butter, that presents an undesirable white phase on it as aging goes on. Domains produced by this white phase are fractal-like and are related with a phase transition... or not. This is a beautiful example of a process near equilibrium but complicated enough to doubt about effectiveness of an equilibrium approach to understand it. Finally, I will briefly depict the problem to design a biomaterial based on collagen and the way that kinetics matter as much as equilibrium properties to succeed in the design.

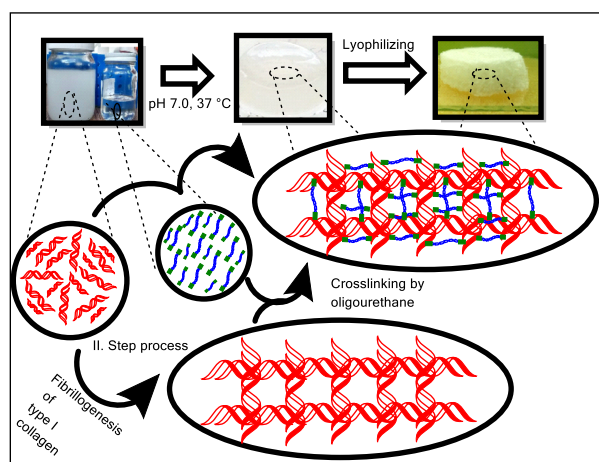


Figure [1]: Outline of the preparation of hybrid hydrogels based on hydrolyzed extracellular matrix and water-soluble oligourethanes showing the aspect of liquid precursors (top left), hydrogel (top center) and sponge (top right). The gel can be formed by simultaneous process or by step process as figure depicts.

**From ballistic to diffusive motion in granular matter**

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Single particle motion in a two-dimensional granular system is investigated in the time range from ballistic to diffusive. The system consists of 1 mm stainless balls on a plane circular surface. The motion of the particles is produced by an alternating magnetic field applied perpendicular to the surface of the container. The mean square displacement of the particles is measured for a range of low concentrations. It is found that increasing the concentration of particles maintaining all other conditions constant is equivalent to do a zoom out in both the spatial and temporal dimensions and in this way one can access the full range from ballistic to diffusive motion and to obtain details of the motion at different instances. A comparison with the solution of the Langevin equation for the mean square displacement of a single particle in a thermal bath shows an excellent agreement for the full time range.



## **General overview of glassy dynamics and arrested states in binary mixtures of hard-spheres: dynamical decoupling, mixed states and bifurcation.**

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The fundamental description of dynamically arrested states of matter is a crucial step towards understanding, and ultimately controlling, the properties of many materials with relevance in biophysics, biotechnology, food science, drug delivery, and other related areas of research with high technological impact. Such is the case of glasses, gels and other *amorphous* solids with which we also have a common daily interaction. In this regard, model colloidal suspensions have played a significant role towards understanding dynamical arrest. Among a wide range of model colloidal systems, the asymmetric binary mixtures of hard-spheres belong to an important class of soft matter materials able to display a rich variety of dynamically arrested states, ranging from repulsive glasses, gels, mixed states and attractive glasses which are far from being completely understood. In this contribution, combining molecular dynamics simulations and theoretical calculations, together with available experimental data, we report a general overview of the various arrested states occurring in a largely-asymmetric binary mixture of hard-spheres. We discuss the fundamental relevance of considering the dynamics of both species in the description of the whole dynamical arrest phenomena. Our findings suggest that, depending on the molar composition and total concentration, the density correlations of each species exhibit different decay patterns and noticeable decoupling effects which become larger near the glass transition. In particular, we suggest the existence of three different transition lines describing distinct glassy phenomena, but converging at a high order singularity in the parameters space of the system.

**Depletion forces in a confined 2D bidisperse WCA fluid**

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We show how to measure depletion forces for a bidisperse fluid of hard disks confined in a channel, interacting via the repulsive Weeks-Chandler-Andersen potential. At a given time, the total force acting over a large disk is assumed to be a combination of the nude force between large disks and an effective force mediated by the small disks, plus a noise term. We use Least Squares over a large number of realizations of this force combination in order to separate the effective forces from the noise. We are able to obtain a depletion force between large disks, and also between large disks and walls. We find that the disk-disk depletion force shows little or no sensitivity to the distance to the walls. We also calculate the anisotropic structure factors, that can be used in the future to test, via a one-component simulation, the quality of the results.

## Dynamic transition and memory encoding in glass-formers under shear

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Understanding the behavior of glasses under mechanical deformation is of primary importance in applied science and, at the same time, it still presents a major problem for basic science. As a matter of fact, while the deformation behavior of crystals is theoretically well understood, no universally accepted framework exists to rationalize mechanically driven amorphous systems. I will present some recent numerical work on the strain deformation of a model glass former under periodic shear deformations. I will show that after a transient, the glass enters a stationary state whose nature depends dramatically on the amplitude of the deformations. For large amplitudes, the system will be diffusive, but below a certain threshold it will enter a cyclic orbit in phase space and the system will be not diffusive [1]. Interestingly, since the non-diffusive state is also non-ergodic, it retains memory of its initial stage and this fact can be used to store and read information by a simple shear protocol [2]. Both the dynamic transition and the memory effects discussed here have a strong analogy to what have been observed in sheared dilute suspensions [3,4]. This is a quite surprising result given the profound differences between the two systems. I will try to rationalize such universal behavior with the help of few toy models [5].

[1] D. Fiocco, G. Foffi, and S. Sastry, Phys. Rev. E, 88, 020301, (2013).

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[3] L. Cort, P. Chaikin, J. Gollub, and D. Pine, Nat. Phys., 4, 420, (2008).

[4] N. C. Keim and S. R. Nagel, Phys. Rev. Lett., 107, 010603, (2011).

[5] D. Fiocco, G. Foffi, and S. Sastry, Journal of Physics: Condensed Matter 27 (19), 194130 (2015)

## Out-of-Equilibrium Assembly of Colloidal Particles at Air/Water Interface Tuned by Their Chemical Modification

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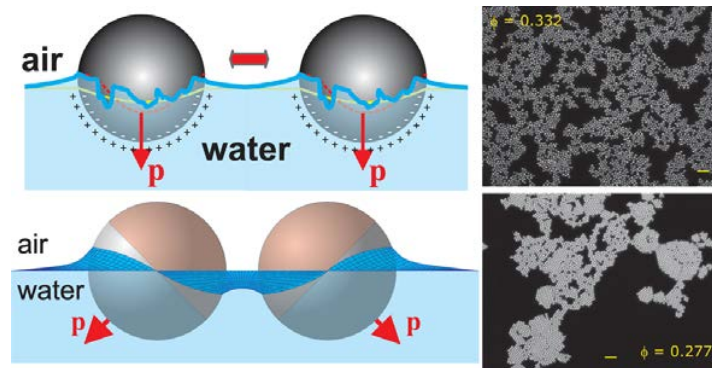
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**ABSTRACT:** Assemblies of monolayers made of colloidal silica particles trapped at the air/water interface are prepared to have an increasing capillary interaction. Fine-tuning of the strength of interaction and its orientational specificity is achieved through isotropic or anisotropic colloid surface chemical modification or by adjusting the subphase surface tension. The capillary attraction between colloids is strong and specific enough to drive the particle organization out of equilibrium toward kinetically arrested assemblies. For isotropic particles, the square order competes with the hexagonal one at low area densities, which leads to their mutual frustration resulting in a polycrystalline solid at high densities. Anisotropic Janus particles attract so strongly and with such an orientational specificity that the resulting assemblies are the most dynamically arrested, although the crystal grains are highly ordered on the short length scale. We show that the particle anisotropic surface modification does not always result in a good long-range ordering at interfaces, although it opens up new possibilities of structure control.



**Abstracts:**

**Contributed Talks**

## Phase behaviour of attractive microswimmers

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Microorganisms live in aqueous environments and their interaction among them and with the fluid becomes a key feature to understand the transport of chemical substances, energy and momentum in many biological, medical and engineering phenomena. Microorganism suspensions are intrinsically out of equilibrium, since they put/consume energy to/from the system and their collective behaviour emerges from their dynamic self-organization. Such collective behaviour has inspired researchers to deepen the understanding of the physics of motility to engineer complex emergent behaviours in model systems that promise advances in technological applications. I will present a computational study of a model of self-propelled microswimmer suspensions that allows us to identify the basic role that the hydrodynamic coupling through the embedding solvent has in the collective behaviour of such systems. Such a fundamental understanding will help us to identify new routes to design micro-robots that can imitate micro-organisms. Motivated by recent experimental results, I will concentrate on a simplified geometry, where the self-propelled particles move in a quasi-2D geometry. The results show that our simulations can reproduce several regimes of emerging collective behaviour, from isotropic to aligned suspensions; with qualitatively different distributions of cluster-sizes depending on the symmetry of the induced active stresses that characterize the active suspension. In Fig. 1 we summarize all the cases in terms of the hydrodynamic signature that quantifies the active stress ( $\beta$ ) and the relative magnitude of the interaction strength with respect to the active force ( $\xi$ ). Specifically, we have reproduced the living clusters observed by experimentalists for both artificial active colloids and for some types of bacteria.

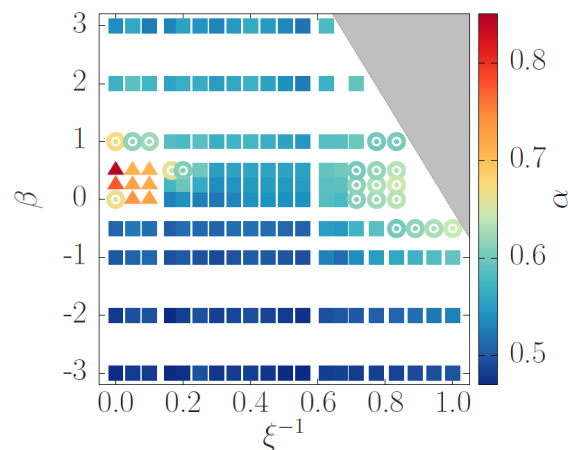


Figure 1: Color map of the scaling exponent  $\alpha$  of the number density fluctuations ( $\langle N \rangle \sim N^\alpha$ ) for homogeneous suspensions. Triangles correspond to giant density fluctuations ( $\alpha > 0.7$ ), circles to an anomalous exponent  $\alpha$  between 0.6 and 0.7, where large fluctuations are observed, and blue squares

**Transport properties of a single nano-colloid from molecular  
dynamics.**

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The motion of a heavy Brownian particle immersed in a medium of lighter particles is described by means of the Generalized Langevin equation (GLE); the latter one can be written as an equation of motion for the time correlation functions of the Brownian particle. The correlation functions are explicitly computed through Molecular Dynamics simulations; they allow one to compute explicitly the memory kernel of the colloidal particle. In particular, we mainly focus on two thermodynamic states of the host medium (high and low temperatures) and four different masses of the nano-colloid. Under such physical conditions, we study the friction and diffusion coefficient of the Brownian particle as function of its mass and diameter to test the Stokes-Einstein relation and discuss the application of the Kirkwood definition for the friction coefficient.

**Visualization of membrane of E. Coli using deconvolution in  
brightfield and fluorescence**

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We obtained images in brightfield and fluorescence of cells of E. Coli and using an experimental Point Spread Function (PSF) in brightfield and a theoretical Point Spread Function in fluorescence we show that the two methods give us the same shape and size of the cell of E. Coli. Applying the deconvolution method and using both PSF in our images obtained experimentally, we give a useful and easy way to enhance images and define better the contour and size of the cell.



## On the motion of carbon nanotube clusters near optical fiber tips: effects of thermal convection and thermophoresis

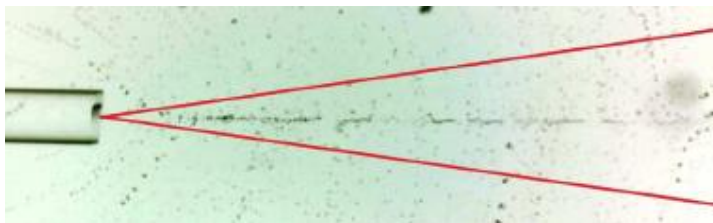
J. Rodrigo Vélez-Cordero<sup>a\*</sup>, J. Hernández-Cordero<sup>b</sup>

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Phoretic transport is defined as the movement of colloidal particles by a field that interacts with its surface. Here we show that multiwalled carbon nanotube clusters (mWCNT-clusters) interact with a laser beam forming a well ordered cluster aligned with the beam axis (see Figure 1). Three main actors were thought to contribute to the observed motion (mWCNT-cluster velocities of the order of 25 $\mu$ m/min): thermal convection effects, optical trapping and thermophoresis.



**Figure 1:** Superimposed images showing the mWCNT-cluster displacements in ethanol upon irradiation with a 975nm laser beam guided by an optical fiber (125 $\mu$ m in diameter). The red lines are guides to the eye and denote the divergence of the laser cone, calculated as  $\sin^{-1}[0.14/n]$ , 0.14 being the numerical aperture of the fiber and  $n$  the refractive index of the fluid.

Thermal convection effects were estimated by solving the Stokes and heat transfer equations numerically (finite element, COMSOL). Optical gradient forces were estimated, on the other hand, considering a Gaussian intensity profile and the polarizability of carbon nanotube arrays. We found the former to be much more relevant than the later upon comparing with experimental data. In order to account for thermophoretic effects, we followed an approach close to [1,2] in which a microscopic momentum balance is made around a colloidal particle taking into account a particle-solvent interaction potential in the context of a thin film approximation. The final equation gives the right direction and magnitude of the experimental velocity if one considers a repulsive interaction potential between the mWCNT-clusters and the polar solvent (hydrophobic interactions).

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**Stress distribution in two-dimensional silos**

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Simulations of a two-dimensional silo were performed with different numbers of grains reaching up to 64 000, verifying numerically the model derived by Janssen and also the main assumption that the walls carry part of the weight due to the static friction between grains with themselves and these with the silo's walls. We vary the size of the silo's bottom, the friction coefficient, and the polydispersity. We find that both the friction coefficient and the size of the silo's bottom change the Janssen's parameter  $K$ , indicating that the assumption that  $K$  is constant with the system geometry is incorrect. Likewise we get the normal force on the walls evidencing the existence of points of maximum stress in the middle of the silo's height.

# Semiflexible curves under confinement or affected by environmental conditions

Dulce Maria Valencia M.

August 1, 2016

## **Abstract**

The confinement of semi-flexible polymers or filaments by curved surfaces is increasingly recognized to be a key element in a number of physical processes happening in systems such as DNA actin filaments, microtubules or linear protein complex that self-assembles on some surfaces. Resistance to bending becomes relevant in the modeling of those systems, on the appropriate length scale. However the behavior of an elastic curve substrate bound or under confinement will reflect the geometry of its surface background in which it is bound or contained. Since in those problems the environment will play a role, there is no single physically relevant analogue of the Euler elastic bending energy of a space curve, quadratic in the three-dimensional Frenet curvature along the curve. We present here a formalism to deal with a generalized bending energy, that can describe the above mentioned situations, and we determine the Euler Lagrange equations, that will describe the equilibrium states of a system with the appropriate boundary conditions. Moreover we can get the forces and torques that are required to sustain a particular configuration.

## The discontinuous ideal glass transition, a soft crossover at finite waiting times.

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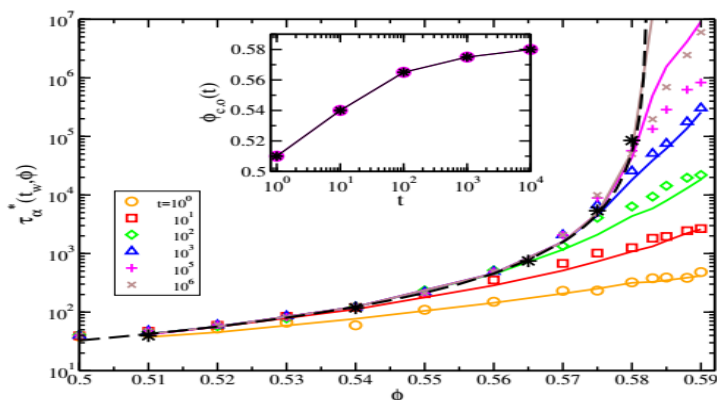
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The non-equilibrium self-consistent generalized Langevin equation (NE-SCGLE) theory of irreversible processes in liquids is shown to provide a coherent and conceptually simple picture of the crossover from ergodic equilibration to non-equilibrium aging in structural glass-forming liquids. According to this picture (see Figure 1), the glass transition is in essence a discontinuous, “mode-coupling”-like transition, characterized by the abrupt passage from ergodic to dynamically arrested states and by the divergence of the equilibrium  $\alpha$ -relaxation time at the transition. The same picture, however, also predicts that such discontinuous and singular scenario will be blurred in real life by the unavoidable finiteness of the time window of any experimental observation.



**Figure 1:** Non-equilibrium Molecular Dynamics simulations (symbols) and NE-SCGLE theoretical results (solid lines) for the  $\alpha$ -relaxation time scaled as  $\tau_\alpha^*(t_w, \phi) \equiv k^2 D_0 \tau_\alpha(k\sigma; t_w, \phi)$  for  $k\sigma = 7.1$ , plotted as a function of  $\phi$  for fixed times  $t = 10^0, 10^1, 10^2, 10^3, 10^4$  and  $10^5$  (from bottom to top; the dashed line corresponds to  $t = \infty$ ). In this case, the dark asterisks indicate the (theoretical)  $t$ -dependent volume fraction  $\phi_{c.o.}(t)$  that describe the crossover from fully equilibrated to insufficiently equilibrated conditions. In the inset we compare the predicted (asterisks) and simulated (circles) results for  $\phi_{c.o.}(t)$ .

**2<sup>nd</sup> International Workshop on Matter Out of Equilibrium,  
22-26 August 2016, Guanajuato, México**

The first systematic comparison of these predictions with pertinent results of the molecular dynamics (MD) simulations[1], involving a polydisperse hard-sphere (HS) liquid, is explained briefly in this talk. To model the polydispersity as well as the passage from short-time ballistic to long-time diffusive dynamics involved in these MD simulations here we resort to the molecular (not Brownian) version of the recently-developed multicomponent NESCGLE theory[2]. As shown in Figure 1, within the time window of the simulations, a remarkable quantitative agreement is observed between the predicted scenario and the simulation results.

[1] G. Pérez, et al., Phys. Rev. E **83**, 060501(R) (2011).

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## Equilibrium and non-equilibrium states in binary mixtures

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The colloidal systems belong to the class of soft materials that have been having a growing interest as ideal model systems for the study of equilibrium and non-equilibrium properties of matter. From a fundamental point of view, these systems present multiples phase transition scenarios, each of one's depending of the kind of interaction between the particles (i.e. the changes of control parameter like Temperature, density, etc.) represent a fascinating research area by itself. For example, it is well known from experimental and simulations studies that a simple mixture of colloidal hard spheres and non-adsorbing polymer shows multiples dynamics arrest scenarios, enriching its equilibrium phase diagram. The same occurred in a mixture of charged particles, where the people have been found interesting scenarios about nucleation, spinodal decomposition, aggregation and gelation. In this work we present a theoretical study of several models of binary mixture, namely: the hard sphere, the soft sphere and the Asakura-Oosawa binary mixture. We draw the dynamic arrest phase diagrams and we present results about the dynamic properties using for this propose the Non-Equilibrium Self Consistent Generalized Langevin Equation theory (NE-SCGLE). Finally, we compare some of our theoretical predictions with simulations results made for each binary mixture model.

**Light absorbing scattering techniques in soft matter**

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There exist different micro-rheological techniques for studying the structural and dynamical properties of complex fluids at a supramolecular level. Among these we find the light scattering techniques: Dynamic Light Scattering (DLS) [1] and Diffusing Wave Spectroscopy (DWS) [2]. Both of them work as a complementary technique of the other one, in this case because we can get a wider landscape of the viscoelastic spectrum of the studied systems. These light scattering techniques take advantage of the Brownian motion of probe particles embedded into the fluid, which scatter the incident light in all directions. Retrieving the scattered light, it is possible to estimate the mean square displacement of the particles (MSD) by means of the correlation function generated by the photons that reach the detector.

It is important to note that the fluid medium to be analyzed should be transparent to the incident light, but using a recent technique developed by Prahl [3] for medical applications and studied and applied by Sarmiento-Gómez et al [4], it is possible to extend the DWS technique to light absorbent fluids. This technique also allows the possibility of extent in time the MSD response, becoming a complementary technique when backscattering DWS is difficult to set up.

In this work we show some preliminary microrheological results of a system of worm-like micelles made by the self-assembly of 1, 4 poly (1, 3-butadiene)-polyethylene oxide diblock copolymer in water solution [5] and preliminary rheological results of a system of single wall carbon nanotubes (SWNT) dispersed in Poly(acrylic acid) as a function of a variation of its pH [6].

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[2] D. Pine, et al., *J. Phys. France*, **51**, 2101-2127 (1990).

[3] S. A. Prahl, et al., *Applied Optics*, **32**, 4 (1993).

[4] E. Sarmiento – Gomez, et al., *Applied Optics*, **53**, 21 (2014).

[5] B. Arenas-Gómez, et al., *Eur. Phys. J. E*, **37**, 51 (2014).

[6] C. Zakri et al., *Langmuir*, **25**(22), 13206–13211 (2009).

**Thermodynamic properties of 1:1 electrolyte solutions in the  
Statistical Associating Fluid Theory plus Binding in the Mean  
Spherical Approximation Theory**

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Given the technological relevance of electrolyte solutions in various branches of science and technology, several theoretical models in literature have been proposed to give insight on structural and thermodynamic properties of systems of charged particles in an aqueous media, presenting association and dissociation phenomena such that they deviate strongly from ideal liquid behaviour.

No exact analytical theory can be developed due to the long range nature of the ionic interactions, so several analytical approximations are to be made in order to accurately describe properties of interest. One of such models is the SAFT-VRE approach (Statistical Associating Fluid Theory for Potentials of Variable Range in Electrolyte Solutions): this approach incorporates several contributions describing monomeric interaction, associating interaction and ionic contributions, and has been successfully applied to the calculation of osmotic pressures and mean activity coefficients for several electrolyte solutions. In order to improve the approximations used in the calculation of the ionic contribution in this model, we propose the use of analytical expressions derived from the BiMSA (Binding in the Mean Spherical Approximation) theory, which has been reported as an accurate description of ionic association and electrostatic phenomena contributions to osmotic and activity coefficients.

In this work we apply the ionic contributions to the EOS of the system from the BiMSA theory within the theoretical SAFT-VRE approach, and compare our predictions with experimental data available for electrolytes 1:1 of osmotic coefficients. We discuss the improvements of this theoretical model and propose how to implement it for multiple valence electrolytes.



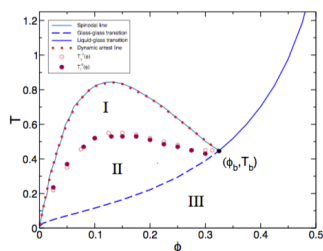
## Formation of amorphous solids by arrested spinodal decomposition

J. M. Olais-Govea<sup>\*a</sup>, L. López-Flores<sup>a</sup> and M. Medina-Noyola<sup>a</sup>

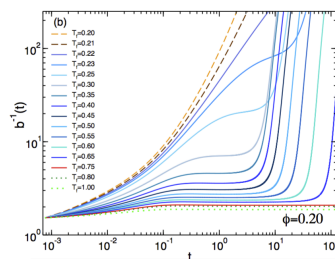
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The non-equilibrium self-consistent generalized Langevin equation (NE-SCGLE) theory of irreversible relaxation [1,2] is applied to the description of the non-equilibrium processes involved in the spinodal decomposition of suddenly quenched simple liquids. For significantly deep quenches, the spinodal decomposition may be interrupted by the dynamic arrest of the condensed phase. This interruption results in the formation of amorphous solids (e.g. gels, porous glasses, etc.), characterized by aging effects and a strong dependence on the preparation protocol. Determining the molecular origin of this phenomenon, referred to as arrested spinodal decomposition, is only one aspect of the more general challenge of understanding glasses, gels and other non-equilibrium amorphous solids. The present work is aimed specifically at understanding the glass and the gel transitions in colloidal systems modelled by hard-sphere plus attractive pair potential. Here we explain the predicted NE-SCGLE scenario, summarized by a rich phase diagram [3] that includes the border lines of gels and porous glasses at low densities and temperatures because of arrested spinodal decomposition (see Fig. 1) as has been experimentally reported [4]. This complex scenario is confirmed by the kinetics of the formation of these arrested disordered structures: for a sudden quench to a temperature  $T$  below the spinodal temperature  $T_S$ , the  $t_w$ -dependence of the mobility function  $b(t_w; T)$  exhibits the appearance of a latency time (the duration of the plateaus in Fig. 2) in which the system seems to equilibrate before dynamic arrest actually sets in. This latency time  $t_l(T)$  is predicted to diverge as  $t_l(T) \sim (T_S - T)^{-2.5}$  as the final temperature  $T$  of the quench approaches the spinodal temperature from below in agreement with experimental observations [5, 6].



**Figure 1:** Non-equilibrium phase diagram of the liquid of hard-spheres of diameter  $\sigma$  with Yukawa tail attraction (of inverse decay length  $z=2/\sigma$ ) in the temperature-volume fraction plane  $(T, \phi)$ , predicted in Fig 10 of Ref. [3].



**Figure 2:** Mobility function  $b(t_w; T)$  as a function of waiting time  $t_w$  for a sequence of quenches along isochore  $\phi=0.2$  to the indicated final temperatures  $T$ .

- [1] P. Ramírez-González and M. Medina-Noyola. *Phys. Rev. E*, **82**(061503), 2010.
- [2] P. Ramírez-González and M. Medina-Noyola. *Phys. Rev. E*, **82**(061504), 2010.
- [3] J. M. Olais-Govea, L. López-Flores and M. Medina-Noyola. *J. Chem. Phys.*, **143**(174505), 2015.
- [4] T. Gibaud and P. Schurtenberger. *J. Phys. Cond. Matter* **21**(32201), 2009.
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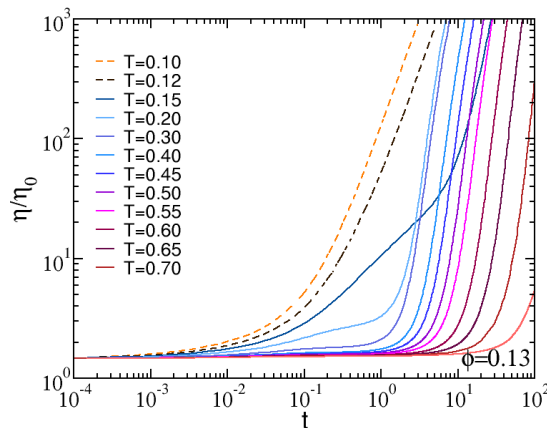
## Linear viscoelasticity on arrested spinodal decomposition

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The recent non-equilibrium self-consistent generalized Langevin equation (NE-SCGLE) theory of irreversible process in liquids [1,2] has permitted to obtain a description of non-equilibrium processes involved in the arrested spinodal decomposition due to sudden and deep quenches inside the spinodal region. For a simple model liquid, where the system could be modeling by a hard sphere plus an attractive Yukawa tail, this theoretical approach predicts that the spinodal line is the borderline between the ergodic and the arrested states. Also, by means of this approach has been determined a border between phase separation and gelation, besides providing the corresponding dynamic properties to each phase [3]. This work addresses a general method to obtain the linear viscoelastic properties of non-equilibrium processes involved in the spinodal decomposition when the system has been quenching inside the spinodal region. In the Fig. (1), we show an example of the normalized shear viscosity as a function of the waiting time. This scheme offers the opportunity to describe the linear viscoelasticity and the diffusion mechanics as the waiting time elapses. Furthermore this approach is able to describe gelation effects, it leads naturally to a diverging shear viscosity at glass and gelation transition points.



**Figure 1:** Behavior to the normalized shear viscosity without HI for hard sphere system plus attractive Yukawa tail (the inverse of the screen parameter  $z=2$ ) for different deep quench, inside the spinodal line.

- [1] P. E. Ramírez-González and M. Medina-Noyola, Phys. Rev. E 82, 061503 (2010).
- [2] P. E. Ramírez-González and M. Medina-Noyola, Phys. Rev. E 82, 061504 (2010).
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## Complexity of a system of non-vibrational steel beads under a time-dependent magnetic field

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<sup>a</sup> Cátedras Conacyt- Instituto de Física, Universidad Autónoma de San Luis Potosí, Álvaro Obregón 64, 78000 San Luis Potosí, S.L.P., México., Times New Roman, 11, italic

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We study the structural properties of a glass former model based on non-vibrating steel beads subjected to an alternating magnetic field. In this system, the particles remain on the plane, in contrast to the vibratory systems where the particles move also in the vertical direction. We determine the radial distribution function and the fractal dimension and found that as particle concentration increases, properties similar to that observed near a glass transition were observed.

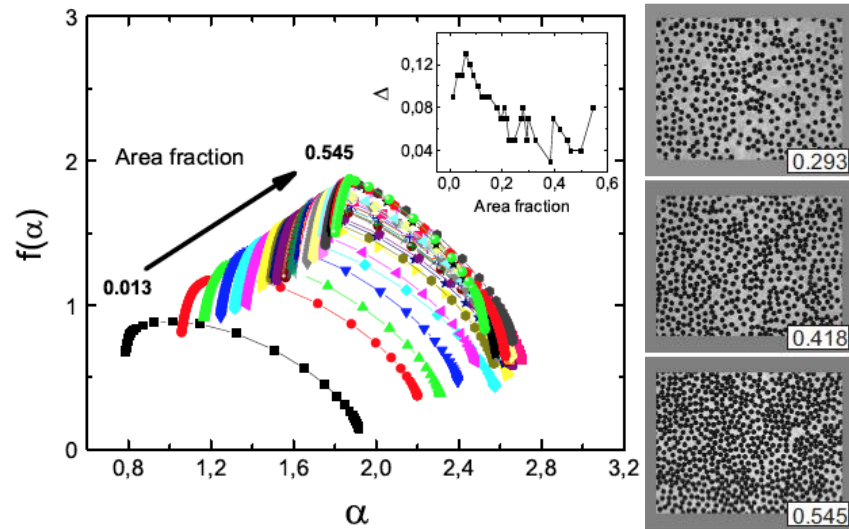


Figure 1: Singularity spectrum for different concentrations of the steel bead system. Inset: the singularity width for the same concentrations

- [1] A.B. Chhabra, C. Meneveau, R. V. Jensen, and K.R. Sreenivasan, *Phys. Rev. A*, **40**, 5284 (1989).
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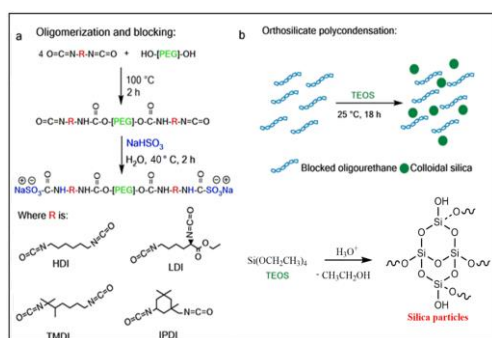
## Modified collagen gel networks: preparation and biomedical applications

Birzabith Mendoza Novelo

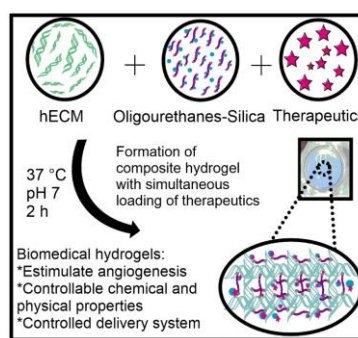
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Type I collagen consists of chains with  $(\alpha 1)2\alpha 2$  molecular formula arranged mostly in the form of a triple helix. This biopolymer can be extracted from mammalian tissues and afterward can be polymerized to form a 3D gel network. The common polymerization of collagen in response to change of pH and temperature is easily combined with the modification with water-soluble oligourethanes and dispersed silica particles [1-2]. The difference in reactivity and steric constraints of diisocyanates as well as in functionality number of poly(ethylene oxide) enable the control of the chemical structure of silica-oligourethane species, as schematized in figure 1. Consequently, the oligourethane molecular size and structure determines the silica-precursor polycondensation and the simultaneous collagen crosslinking. Properties of the hybrid gel network, such as swelling, biodegradation, mechanics, are therefore tailored to match with the specific requirements of the biological applications (figure 2). In this regard, these engineered hydrogels have shown promising characteristics as system for controlled delivering of therapeutics and for inducing the cell fate, as it will be described in the workshop.



**Figure 1:** Scheme of the preparation of crosslinkers composed of silica-oligourethanes. a) Synthesis of aqueous oligourethanes from PEG (1000 g mol<sup>-1</sup>) and different aliphatic diisocyanates. b) TEOS condensation to disperse colloidal silica particles in the oligourethane solution.



**Figure 2:** Schematic illustration of the formation of biocomposite hydrogels as controlled release systems of therapeutics.

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## Sedimentation of Particles in Viscoelastic Fluids

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We use a phenomenological model to discuss the complex rheology of glass-forming (viscoelastic) liquids by incorporating interaction between slow relaxation and flow induced rearrangements in the fluid [1]. A Maxwell-type constitutive equation is introduced to define the non-Newtonian stress tensor ( $\boldsymbol{\sigma}$ ) and close the Navier-Stokes equations:

$$\dot{\boldsymbol{\sigma}}(t) = G_{\infty} D(t) - f(\vec{r}, t) \boldsymbol{\sigma}(t) \quad (1)$$

where the local relaxation rate  $f(\vec{r}, t)$  is called fluidity [2] and obeys a diffusion-relaxation equation:

$$\partial_t f(\vec{r}, t) = -\frac{1}{\tau_f} \left( f(\vec{r}, t) - \frac{1}{\tau_M(\dot{\gamma}(t))} \right) + \frac{\xi^2}{\tau_f} \Delta f(\vec{r}, t) \quad (2)$$

Shear thinning effects are included by setting  $1/\tau_M = 1/\tau + |\dot{\gamma}|/\gamma_c$ , where  $\dot{\gamma}$  is the local flow rate. Diffusion term  $\xi^2/\tau_f \Delta f(\vec{r}, t)$  in Eq. 2 accounts for heterogeneities in the flow then we can control how far fluidized regions could spread along their neighbors [2].

We study the flow dynamics of these fluids with particles sedimenting. A resolved method called Fictitious Domain Method (FDM) is used, where forces acting on the surface of the particles are calculated, i.e. no drag models are used [3]. This is done by coupling a Lagrangian Discrete Element Method (DEM) to track the bodies and Computational Fluid Dynamics (CFD) to solve the flow, methodology introduced by [4].

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## Dynamics of shear banding flow in Non-Newtonian fluids.

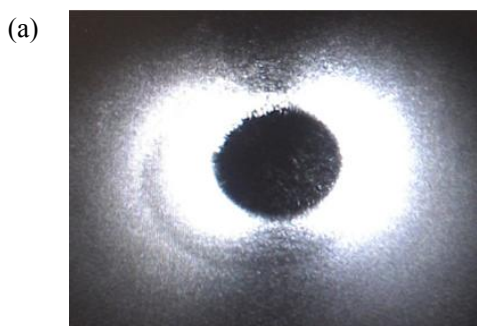
B. L. Arenas-Gómez<sup>a\*</sup>, J. Delgado<sup>a</sup>, A. Tavera-Vazquez<sup>b</sup> and R. Castillo<sup>b</sup>.

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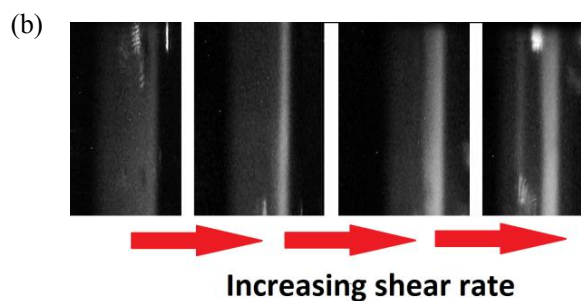
<sup>b</sup> *Instituto de Física, UNAM, Circuito de la Investigación Científica s/n, C.P. 04510, Ciudad de México, México.*

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In this work we try to understand the chaotic flow behaviour of complex fluids in the semidilute regime. We work with three different complex systems which may, or may not, exhibit Maxwellian behaviour. These systems self-assemble, above a critical micellar concentration, in wormlike micelles because their amphiphilic properties, and used to present birefringence under flow. This flow birefringence (or shear banding) is observed by increasing the applied shear rate, which align these wormlike micelles along the direction of the flow. The shear banding is observed using two types of optical rheology, each of them with a different measurement geometry (transparent Couette cell and semitransparent Cone-Plate). Shear banding is a nonequilibrium phenomenon present in some micellar systems where regions of different turbidity coexist under shear, and upon the shear flow cessation this effect is reverted to their transparent state. Previous experiments revealed the existence of fluctuating shear banding flows as the control parameter was increased, and each complex system exhibit different patterns [1,2,3,4]. During a step shear rate experiment in a transparent Couette cell we obtained views of the gap in the plane velocity gradient/vorticity from the recording of the scattered intensity [2]. This allow us to study the spatio-temporal dynamics of the induced band and compare it with their Weissenberg number values and reduced flow curves. We work with these aqueous solutions; TDPS/SDS/NaCl/Water, CTAB/NaSal/Water and PB-PEO/Water.



**Figure 1:** SALS pattern of TDPS solutions under shear (SALS+Reometer).



**Figure 2:** Spatio-temporal evolution of the induced band in TDPS solution at 40 °C.

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**2<sup>nd</sup> International Workshop on Matter Out of Equilibrium,  
22-26 August 2016, Guanajuato, México**

**Runout transition in bidimensional dumbbell-like rock avalanches**

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Experimentally it was found by Bartali et. al. that a flow composed by samples of rocks with small size dispersions, with size classes ranging from 1 mm to 2 cm, show an exponentially increasing behavior in a runout vs particle size plot. Furthermore, these authors showed that this tendency is independent of the amount of falling matter, when it falls from the same height. In the present work we show, using two-dimensional molecular-dynamics simulations, that the runout changes with the amount of matter falling, and that there is a change from an exponentially increasing function to a constant one when we multiply by two the total mass, and moreover, that multiplying again the total mass by two results in an exponentially decreasing behavior. This shows a well defined transition in the runout vs particle size plot when we increase the amount of matter in the avalanche. The main hypothesis to explain this contradictory result is that the change of the transversal length when the flow pass from the flume to the floor zone is not reproducible in a 2D simulation. We also characterize the flow computing the energy and the power dissipated. We show that, although the energy of the avalanche is bigger for smaller particles when the flow is on the flume, these smaller particles dissipate the energy quicker than the big ones when the flow is on the floor. This could be a good explanation for the results obtained by Bartali et. al.



**Long-range effective potential between granular rods within a  
granular medium**

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We present a theoretical calculation of a long-range potential between two rods immersed in a granular medium composed of spheres. Based on previous experimental and numerical works [1], we show the existence of such a potential acting at distances well beyond de classical Asakura-Oosawa depletion potential [2], *i.e.*, distances larger than one sphere diameter ( $\sigma$ ).

We find a layering effect on the surface of the intruders—similar to that found in colloids [3]—generated by a depletion effect, which is enhanced by the inelastic character of the collisions between grains, as well as the Coulomb friction forces. This enhancement provokes a net attractive force between intruders, which can bring them together from long distances, as it has been observed previously in different experiments [1,4].

The calculated potential leads to a long-range distribution function,  $g(x)$  for rods, that can be measured experimentally or numerically, similar to the radial distribution functions measured on granular systems consisting of solely monodisperse spheres [5]. We propose a clustering instability [6] as responsible for this attractive potentials, whose study would help us to understand the segregation phenomena that take place in granular materials.

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- [6] Goldhirsch, I and Zanetti, G. *Phys. Rev. Lett.*, **70**, 1619 (1993).



**Short-time dynamics of monomers and dimers in quasi-two-  
dimensional colloidal mixtures**

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We report on the short-time dynamics in colloidal mixtures made up of monomers and dimers highly confined between two glass plates. At low concentrations, the experimental measurements of colloidal motion agree well with the solution of the Navier-Stokes equation at low Reynolds numbers; the latter takes into account the increase in the drag force on a colloidal particle due to wall-particle hydrodynamic forces. More importantly, we find that the ratio of the short-time diffusion coefficient of the monomer and that of the center of mass of the dimer is almost independent of both the dimer molar fraction,  $x_d$ , and the total packing fraction,  $\phi$ , up to  $\phi \approx 0.5$ . At higher concentrations, this ratio displays a small but systematic increase. A similar physical scenario is observed for the ratio between the parallel and the perpendicular components of the short-time diffusion coefficients of the dimer. This dynamical behavior is corroborated by means of molecular dynamics computer simulations that include explicitly the particle-particle hydrodynamic forces induced by the solvent. Our results suggest that the effects of colloid-colloid hydrodynamic interactions on the short-time diffusion coefficients are almost identical and factorable in both species

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**2<sup>nd</sup> International Workshop on Matter Out of Equilibrium,  
22-26 August 2016, Guanajuato, México**

**Interactions between Liposomes and Nitrogen-Doped Carbon  
Nanotubes: new composites for possible applications.**

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Nitrogen-doped carbon (CN<sub>x</sub>) nanotubes have been synthesized by the aerosol-assisted chemical vapor deposition (CVD) method [1]. Benzylamine was used as nitrogen and carbon precursor and ferrocene as catalyst nanoparticles and the quartz tube as a substrate. The SEM characterization of our samples reveals the formation of carbon nanotubes with different lengths, diameters, and morphologies. Our TEM and HRTEM images show the existence of carbon nanotubes with bamboo-like configurations having carbon-coated iron nanoparticles attached to the external surface, partially buried on the outermost carbon layers, or adsorbed inside the carbon structures[2]. The XPS data reveals i) a N content as large as 2.7 %, ii) the existence of different bonding configurations for the nitrogen species, and iii) that N atoms are distributed all along the carbon nanotubes. Finally, we present preliminary results related to the interaction of our nanotubes with liposome-type structures [3]. The liposomes are composed of mixed molecule DMPC and our nanostructures. TEM imaging shows the formation of composite nanotube/liposome type, which could be used for the design of novel biological conveyors.

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## Equilibration and Aging of Liquids of Non-Spherically Interacting Particles

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In this work, we present a first step in the direction of extending the NE-SCGLE to describe the irreversible evolution of the static and dynamic properties of Brownian liquids made up of particles with non-radially symmetric interactions, where the simultaneous description of translational and orientational degrees of freedom is essential. The theory consists of the coarse-grained time-evolution equations for the spherical harmonic projections of the structure factor of the fluid, which involves both translational and rotational time-dependent mobility functions. This theory is able to model the irreversible processes occurring after a sudden temperature quench, where the spontaneous time evolution of the system might lead to two possible, and mutually exclusive, physical scenarios, namely: equilibration, or aging of the dynamics, due to the emergence of conditions of dynamical arrest for either translational or orientational (or both) degrees of freedom. We illustrate the predictive capability of our theoretical approach by applying the resulting equations to the description of the orientational relaxation of a dipolar hard sphere fluid with fixed random positions, after being subjected to an instantaneous temperature quench.

**Assessment of the micro-structure and depletion potentials in two-dimensional binary mixtures of additive hard-disks**

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Depletion forces are a particular class of effective interactions that have been mainly investigated in binary mixtures of hard-spheres at the bulk. Although there are a few contributions that point toward the effects of confinement on the depletion potential, little is known about such entropic potentials in two-dimensional colloidal systems. From theoretical point of view, the problem resides in the fact that there is no a general formulation of depletion forces in arbitrary dimensions and, typically, any approach that works well in three dimensions has to be reformulated in lower dimensions. However, we have proposed a theoretical framework, based on the formalism of contraction of the description within the integral equations theory of simple liquids, to account for effective interactions in colloidal liquids, whose main feature is that it does not need to be readapted to the problem under consideration. We have also shown that such approach allows one to determine the depletion pair potential in three-dimensional colloidal mixtures even near to the demixing transition provided the bridge functions are sufficiently accurate to correctly describe the spatial correlation between colloids [1]. We here report an extensive analysis of the structure and the entropic potentials in binary mixtures of additive hard-disks. In particular, we show that the same functional form of the modified-Verlet closure relation used in three-dimensions can be straightforwardly employed to obtain an accurate solution for two-dimensional colloidal mixtures in a wide range of packing fractions, molar fractions and size asymmetries. Our theoretical results are explicitly compared with the ones obtained by means of event-driven molecular dynamics simulations and recent experimental results. Furthermore, to assess the accuracy of our predictions, the depletion potentials are used in an effective one-component model to reproduce the structure of the big and the small disks. This demonstrates the robustness of our theoretical scheme even in two dimensions.

[1] Erik López-Sánchez, César D. Estrada-Álvarez, Gabriel Pérez-Ángel, José Miguel Méndez-Alcaraz, Pedro González-Mozuelos, and Ramón Castañeda-Priego, *J. Chem. Phys.* **139**, 104908 (2013).

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