

Challenges in Nonlinear Systems: A meeting to celebrate the 60th birthday of Prof. L.L. Bonilla

Leganés July 6–7, 2017

Thursday, July 6

Aula de Grados

09:00-09:15 Opening ceremony

09:15-09:45 Amable Liñan (UPM): TBA

09:45-10:15 Stephanos Venakides (Duke) Lossless Polariton Solitons

10:15-10:45 John C. Neu (Berkeley) Stochastic ODE Theory of Heat Transfer

10:45-11:15 Coffee break

11:15-11:45 Holger T. Grahn (PDI, Berlin) Why are weakly coupled semiconductor superlattices chaotic?

11:45-12:15 Stephen W. Teitsworth (Duke) Noise-induced transitions in nonlinear electronic transport structures

12:15-12:45 José Javier Brey (US) Kinetic equation for a confined quasi-two-dimensional gas of hard spheres

12:45-13:15 J. Miguel Rubi (UB) Casimir forces out of equilibrium

13:15-14:30 Lunch

14:40-15:00 Carlos A. Velasco (FIT Bonn) Using Machine Learning to address social challenges

15:00-16:00 Poster session

Room 4.1.E01

16:00-16:30 Inmaculada R. Cantalapiedra (UPC) Mechanisms underlying electro-mechanical cardiac alternans

16:30-17:00 Antonio Prados (US) Spin-string and spin-membrane models: A mesoscopic approach to rippling and buckling in graphene

Friday, July 7

Aula de Grados

09:30-10:00 Daniel Rodríguez (UNED)

How chemo-radiotherapy may be modeled with simple statistical mechanics rules?

10:00-10:30 Pedro L. García Ybarra (UNED) Near-wall turbulent transport of large Schmidt number passive scalars

10:30-11:00 José L. Castillo (UNED) Electrospraying deposition of nanoparticles

11:30-12:00 Coffee break

12:00-12:30 Antonio Marquina (UV) Non-convex relativistic flows under a phenomenological equation of state

12:30-13:00 Francisco J. Higuera (UPM) Analysis of the flow in a pressure swirl atomizer

13:00-13:30 Andrés Santos (UNEX) Granular gases as a paradigm of the Mpemba effect

13:30-15:00 Lunch

15:00-16:00 Poster session

Room 4.1.E01

16:00-16:30 José M. Vega (UPM) Higher Order Dynamic Mode Decomposition

16:30-17:00 Gloria Platero (ICMM-CSIC) Two Qubit Manipulation with Driven Fields

17:00-17:15 Closure ceremony

Kinetic equation for a confined quasi-two-dimensional gas of hard spheres

J. Javier Brey¹

¹Departamento de Física Atómica, Molecular y Nuclear, Universidad de Sevilla, Sevilla, SPAIN

A system of hard spheres enclosed between two infinite horizontal parallel plates, separated a distance between one and two particle diameters is considered in the dilute limit. A Boltzmann-like kinetic equation is derived. The equation incorporates the effect of the confinement on the possible collisions. A Lyapunov entropy function is constructed by adding to the Boltzmann expression a confinement contribution. The expressions for the steady entropy and density profiles are derived and showed to agree with previous results derived by means of equilibrium density functional theory. The theoretical predictions are compared with molecular dynamics simulation results, and a good agreement is found. As a first application, evolution equations or the vertical and horizontal temperature parameters are derived and their solutions again compared with simulation results. The relevance of the model to analyze some experimental observations in granular gases is discussed.

Mechanisms underlying electro-mechanical cardiac alternans

Inmaculada R. Cantalapiedra¹

¹Departament de Física Aplicada, Universitat Politècnica de Catalunya, Barcelona, SPAIN

Electro-mechanical cardiac alternans consists in beat-to-beat changes in the strength of cardiac contraction. Despite its important role in cardiac arrhythmogenesis, its molecular origin is not well understood. The appearance of calcium alternans has often been associated to fluctuations in the sarcoplasmic reticulum calcium level (SR Ca load). However, cytosolic calcium alternans observed without concurrent oscillations in the SR Ca content suggests an alternative mechanism related to a dysfunction in the dynamics of the ryanodine receptor (RyR2). In this talk we review recent results regarding the relative role of SR Ca content fluctuations and SR refractoriness for the appearance of alternans in both ventricular and atrial cells.

Electrospraying deposition of nanoparticles

J.L. Castillo,¹ S. Martín,¹ Daniel Rodríguez-Pérez,¹ and P.L. Garcia-Ybarra¹

¹Dept. Fisica Matematica y de Fluidos, UNED. Senda del Rey 9, 28040 Madrid, SPAIN

Aerosol technologies have increased their application field ranging from environmental issues of social concern to the fabrication of new materials with specific properties. The distinctive large surface/volume (surface/mass) ratio of aerosols made them especially suitable for procedures requiring a large active surface area which is the case for catalyst applications, solvent fabrication or pharmaceutical products. Moreover, aerosol nanoparticles can be used as building blocks for preparation of new materials which still retain this large surface/volume ratio as their distinctive feature. Many practical applications make use of porous materials and suitable values of surface roughness and bulk porosity may be required. In this sense, the deposition of electrosprayed suspensions of nanoparticles leads to porous films whose morphological properties may be controlled by adjusting the electrospray parameters.

An experimental work is being carried out to perform a broad study of deposit features as a function of electrospray working conditions. A suspension of carbon nanoparticles in ethanol is steadily electrosprayed in the cone-jet mode with the resulting charged droplets driven towards a collecting surface. Ethanol evaporates during the droplet flight and the particles emitted at the electrospray tip are collected on the substrate building up a granular deposit of nanoparticles. Depending on the electrospray operating conditions, aggregates or even single catalyst particles can reach the substrate generating a dendritic-like and highly porous deposit. Changes in the liquid composition and in the electrospray working parameters (needle voltage, collector voltage and flow rate) affect the stability of the cone-jet mode and also have a strong influence on the dynamics of particle arrival to the collecting surface which indeed determine the deposit structure.

The deposit morphology has been analyzed as a function of the electrospray flow rate (Q). Carbon deposits were formed with different values of Q but the same total collected mass of nanoparticles. Image processing analysis of SEM images of these deposits allows to determine the mean deposit density. The deposit mean porosity is rather high but decreases with the flow rate showing a transition from dry deposition to wet deposition probably due to incomplete evaporation of ethanol at large enough flow rates.

Near-wall turbulent transport of large Schmidt number passive scalars

P. L. García-Ybarra¹

¹Dept. Fisica Matematica y de Fluidos, UNED. Senda del Rey 9, 28040 Madrid, SPAIN

Turbulent diffusion of a passive scalar with a large Schmidt number (Sc $\gg 1$) is considered in the viscous sublayer of a turbulent channel flow. Close to the wall, the corresponding eddy diffusivity coefficient is expanded as a power series in terms of the viscous distance to the wall y. The coefficients of the series depend on the Schmidt number and the analysis of recent numerical results allows to conclude that, in the close vicinity of the wall ($y \ll$ Sc^{-1/3}), the y³-term is the dominant term whereas, at distances relatively large from the wall (Sc^{-1/3} $\ll y \ll 1$), the y⁴-term becomes dominant. Accordingly, in this region the turbulent Schmidt number is not constant but follows a hyperbolic law in terms of the distance to the wall that matches the values taken in the vicinity of the wall, of order Sc^{-1/3}, with the values of order unity in the rest of the viscous layer. The implications of this behavior on the surface-transfer coefficient are analyzed.

Why are weakly coupled semiconductor superlattices chaotic?

Holger T. Grahn¹

¹Paul-Drude-Institut für Festörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, GERMANY

A weakly coupled semiconductor superlattice represents an almost ideal one-dimensional nonlinear dynamical system with a large number of degrees of freedom, the nonlinearity of which is due to sequential resonant tunneling between adjacent quantum wells. In 1974, this type of superlattice was found to exhibit stationary electric-field domains [1], i.e., an inhomogeneous distribution of the applied electric field with a region of small and a second region of large field strength. In the 1990s, the first indications of instabilities such as current selfoscillations in a weakly coupled GaAs/AlAs superlattice were reported [2]. The oscillatory behavior is attributed to the localized, oscillatory motion of the domain boundary, which separates the high from the low electric-field domain. At the same time, spatiotemporal chaos was predicted to occur in *n*-doped semiconductor superlattices with sequential resonant tunneling as their main charge transport mechanism [3]. Chaos is expected, when the undamped current self-oscillations are driven by means of an external signal. Shortly after, spontaneous, i.e., undriven, chaos was observed in a weakly coupled GaAs/AlAs superlattice at low temperatures [4]. Five years ago, spontaneous chaotic and quasi-periodic current self-oscillations were observed at room temperature in GaAs/(Al,Ga)As superlattices using an Al content of 45% [5], which results in the largest direct barrier for this materials system. Based on these weakly coupled GaAs/Ga_{0.55}Al_{0.45}As superlattices operating at room temperature, an all-electronic true random number generator has been demonstrated [6]. The achievable bit rates of up to 80 Gbit/s are very competitive, being about two orders of magnitude larger than typical bit rates for currently available all-electronic true random number generators. Very recently, the synchronization of chaos based on room temperature spontaneous chaotic current self-oscillations in a weakly coupled GaAs/Ga_{0.55}Al_{0.45}As superlattice has been established as a useful building block for various tasks in secure communications [7]. Finally, last year, noise-enhanced chaos was reported for a doped, weakly coupled GaAs/Al_{0.45}Ga_{0.55}As superlattice at room temperature [8]. It was observed in experiments as well as simulation results of nonlinear transport based on a discrete tunneling model. When the noise amplitude is increased, spontaneous chaotic current oscillations appear over a wider bias voltage range.

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Analysis of the flow in a pressure swirl atomizer

A. Pereña¹ and F.J. Higuera¹

¹E.T.S. Ingenieros Aeronáuticos, Universidad Politécnica de Madrid, Plza. Cardenal Cisneros 3, 28040 Madrid, SPAIN

A pressure swirl atomizer consists of a cylindrical chamber with a convergence and an exit orifice at one end. Liquid is continuously injected into the chamber through tangential orifices near the other end, inducing a swirling flow with an air core along the axis of the chamber. This flow converges towards the exit orifice, in a process that intensifies the rotation, and emerges from the chamber as an annular sheet that rapidly becomes conical. Due to its motion relative to the surrounding fluid, the sheet undergoes a Kelvin-Helmholtz instability that makes it flap and sets the stage for a secondary Rayleigh-Taylor instability that breaks it into ligaments and then drops. Simplified analyses of some of these processes are presented.

Non-convex Relativistic Flows under a Phenomenological Equation of State

Antonio Marquina¹

¹Departamento de Matemáticas, Universidad de Valencia, Valencia, SPAIN

In this work we propose a phenomenological (analytic and very simple) equation of state (EoS) to illustrate the potential effects that a non-convex EoS may produce on both the thermodynamics and the dynamics of relativistic flows. This EoS has the virtue of mimicking the loss of convexity resulting from a non-monotonic behavior of the adiabatic index with density, while at the same time be simple enough to gain a deeper physical insight in a number of phenomena of interest. As we shall see, it is possible to tune the parameters of this phenomenological EoS to emulate the behavior of the sound speed in very dense plasma (above nuclear matter density). The main focus of this work will be to carefully examine the regime in which purely relativistic effects determine the non-convex evolution of prototype relativistic Riemann problems of flows obeying our phenomenological EoS.

Stochastic ODE Theory of Heat Transfer

John C. Neu^1

¹Department of Mathematics, University of California at Berkeley, Berkeley, CA, 94720-3840, USA

A mechanical system with known energy landscape is coupled to various heat baths, possibly of different temperatures. The coupling to heat baths is modeled by overdamping and random forces. The stochastic ODE is a force balance between mechanical forces that derive from the energy landscape, and the bath-derived damping and random forces. So far, a conventional story. If there are differences between bath temperatures, the stochastic ODE violate detailed balance. We calculate heat transfer rates between baths: The statistics of fluctuations is characterized by a second moment tensor. If the mechanical system is on a lattice, like discrete elasticity, you can think of the second moment tensor as a two point corollation function. It satisfies a *fluctuation-dissipation relation*. Knowledge of the second moment tensor is the essential input to compute heat transfer rates between baths. An elementary example is worked out. In nonlinear systems with multiple stable critical points, the heat transfer rates depend on the critical point about which the stochastic trajectory is localized. Intermittant jumps between critical points are then "seen" as jumps in heat transfer rates.

Next, consider two-dimensional lattice field equations which are invariant under discrete translations. If detailed balance holds (all bath temperatures the same, or equivalently, all nodes are coupled to the same bath), the two point corollation function $m(\boldsymbol{x}; \boldsymbol{x}')$ as a function of $\boldsymbol{x}' - \boldsymbol{x}$ is the Green's function of a discrete Helmoltz operator. Breaking detailed balance breaks the translation invariance, and how this plays out in the mathematics is most peculiar: The fluctuation-dissipation relation becomes a discrete Helmholtz equation for $m(\boldsymbol{x}; \boldsymbol{x}')$ in the *four-dimensional space* consisting of $(\boldsymbol{x}', \boldsymbol{x})$ in $\mathbb{R}^2 \times \mathbb{R}^2$. The source term of this Helmholtz equation comes from the lattice points where detailed balance is violated. To date, I've worked out the details for a two-dimensional diode array. By the time of the talk I expect to work out consequences for heat transfer in a mechanical system, such as an elastic lattice.

Two Qubit Manipulation with Driven Fields

<u>Gloria Platero</u>,¹ F. Gallego,¹ and R. Sánchez²

¹Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, SPAIN

²Grupo de Modelización, Simulación Numérica y Matemática Industrial,

Universidad Carlos III de Madrid, Avda. de la Universidad 30, 28911 Leganés, SPAIN

The effect of ac electric fields in the transport properties of low dimensional systems and nanodevices has been a topic of intense research in the last years. Applying ac electric fields to coupled quantum dots allows to control the tunneling between them and to transfer charge by means of photo-assisted transitions. Recent experiments in triple quantum dots unambiguously show direct electron transfer between the outer dots, without the participation of the intermediate region other than virtual, minimizing then decoherence and relaxation. This long range transfer mechanism is mediated by virtual transitions[1,2,3]. In the presence of ac driving the transfer of electrons between distant dots takes place by means of photo-assisted virtual transitions[2,4]. Interestingly, by means of this mechanism, direct transfer of heat and energy between outer dots in a quantum dot array has also been proposed [5].

In the present work we investigate how to manipulate two qubits located at the left and right edges of a triple quantum dot array with two interacting electrons by means of ac gate voltages. Our aim is to transfer a qubit state directly to another distant qubit by means of virtual photoassisted transitions. Our protocol consists first in isolating the two qubits, each in one of the outer dots. The two states of the qubit localized in the left side are connected by a virtual transition through an intermediate state. Once the left qubit is in the desired state, we apply ac gate voltages to the outer dots with amplitudes such that the left qubit state is fully transferred to the right qubit. Furthermore, by manipulating the intensities of the ac voltages we assure that the qubit state is not going to be corrupted by decoherence coming from the mixing of the initial quantum state with other accessible states. Importantly, this decoherence is avoided by the controlled generation of dark-states by the ac gate voltages[4,6]. Our proposal opens a way to transfer quantum states directly between distant regions in solid state devices by means of ac driving fields.

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Spin-string and spin-membrane models: A mesoscopic approach to rippling and buckling in graphene

A. $Prados^1$

¹Física Teórica, Universidad de Sevilla, Apdo. de Correos 1065, Sevilla 41080, SPAIN

In this talk, we discuss some recent work on rippling and buckling of clamped graphene sheets. Specifically, we consider spin-string and spin-membrane models: at each lattice site *i*, the perpendicular to the membrane displacement is modelled by a variable u_i and the remainder of degrees of freedom are embedded in a local pseudospin σ_i [1, 2]. The potential energy of this system has two contributions: (i) an elastic term, coming from the coupling among nearest-neighbour displacements and (ii) an on-site linear spin-displacement term, representing the interaction of the elastic deformations u_i with the internal degrees of freedom σ_i . Our approach is mesoscopic: the system dynamics is introduced as a Markov process for the variables $\{u_i, \sigma_i\}$, with Glauber transition rates for the pseudo-spins.

We show that buckled states appear as a consequence of the coupling among the pseudospins and the elastic variables, below a certain critical temperature [1]. Moreover, if the pseudo-spins have an additional short-ranged antiferromagnetic interaction, there appears a complex phase diagram with rippled and buckled phases [2]. Finally, we explain how recent scanning tunnelling microscopy (STM) experiments with graphene sheets [3], in which a rippled to buckled transition is observed upon local heating, can be understood within the framework of these models [4].

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How chemo-radiotherapy may be modeled with simple statistical mechanics rules?

J. Carlos Antoranz,¹ M^a Mar Desco,¹ and Daniel Rodríguez-Pérez¹

¹Dept. Fisica Matematica y de Fluidos, UNED. Senda del Rey 9, 28040 Madrid, SPAIN

Radiotherapy has been described numerically using different approaches to the effect of radiation on the survival of the malign tissue to be removed. The linear model, first, the linear quadratic model, later, multi-target models, with different corrections to take into account from multiple hits on the DNA, to cell interactions in the tumor, all of them have been proposed based on more or less mechanistic grounds to enhance prediction (or, at least, fit the experimental data).

Some years ago, our group introduced for this complex situation a model inspired by the complex systems thermodynamic theory: A Tsallis' entropy model. This model not only fitted well the available experimental data, or improved usual model predictions at higher dose regimes, but also raised two conjectures: the existence of a critical dose of tissue annihilation (a mathematical requirement!), and the existence of tissue-radiation specific critical exponents (as it had been shown through experimental data analysis). The mathematical structure of the model was later extended to multifractionated radiotherapy, with the only requirement of keeping the dose composition law (simple and) associative. Afterward, the continuous limit, corresponding to brachytherapy, was found to be in accordance with the non-extensive or "deformed" calculus.

These statistical mechanical results have been recently related with a cellular targetlike model in which damage probability is inversely proportional to the number of healthy targets, being the proportionality constant related with the tissue-radiation exponent, and the critical annihilation dose related with the total number of targets (as could be expected). This discretization of the model leads exactly to the statistical mechanics result in the limit of infinitely many targets.

On the other hand, statistical fluctuations in the "cell population" start to play an interesting role when a finite number of targets exists: they cause some high dose effects that prevent an increased efficiency of radiotherapy as found in some types of tumors (as prostate cancer). It is remarkable that this effect does not require further assumptions as needed in other previous models of this effect. The finite-target discrete non-extensive model has also been proposed to describe the interactions between chemo- and radiotherapy, once again keeping the same simple rules derived above, and assuming that some chemopharm agents (such as cisplatin or gemcitabine) do damage the same type of cellular targets (although not exactly the same) as radiotherapy thus acting as chemosensitizers that decrease the critical annihilation dose.

These oversimplified models of radio- and chemo-radiotherapy show how non-extensivity and statistical effects may conspire to produce the wealth of behaviors described in the literature, just using a simple and small set of rules. The model might not be (radio-bio-) physically correct (it is hard to believe it is even a coarse approximation), but all we have learned from it might still be useful.

Casimir forces out of equilibrium

J. Miguel Rubi¹

¹University of Barcelona, Faculty of Physics, Diagonal 647, Barcelona, SPAIN

We analyze both the attractive and repulsive Casimir-Lifshitz forces recently reported in experimental investigations. By using a kinetic approach, we obtain the Casimir forces from the power absorbed by the materials. To this purpose, we consider collective material excitations through a set of relaxation times distributed in frequency according to a log-normal distribution. A generalized expression for these forces for arbitrary values of temperature is obtained [1]. We compare our results with experimental measurements and conclude that the model proposed gives better results than the proximity-force approximation.

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Granular gases as a paradigm of the Mpemba effect

Andrés Santos¹

¹Departamento de Física, Universidad de Extremadura, Badajoz, SPAIN

The Mpemba effect is a counterintuitive phenomenon according to which, given two samples of fluid, the initially hotter one may cool more rapidly than the initially cooler one [1, 2]. A necessary condition for the effect to take place is that the thermal rate of change depends not only on the instantaneous temperature but also on additional variables. In this talk, I will show that the simplest model of a granular gas, both in the uniformly heated and in the freely cooling settings, exhibits a Mpemba effect [3]. By assuming that the most relevant variable to determine the thermal rate of change, apart from the granular temperature itself, is the excess kurtosis of the velocity distribution of the grains, analytical quantitative predictions for how differently the system must be initially prepared to observe the effect are obtained. An inverse Mpemba effect [4] (whereby a cooler fluid heats more rapidly than a hotter one) is also predicted in the case of uniformly heated systems. The theoretical predictions are numerically confirmed by the direct simulation Monte Carlo method and by molecular dynamics. Time depending, it will be shown that the effect is also present in molecular gases subject to a nonlinear drag.

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Noise-induced transitions in nonlinear electronic transport structures

S. Teitsworth¹

¹Department of Physics, Duke University, Science Dr., Box 90305, Durham, NC 27708, USA

Noise-induced transitions between coexisting metastable states occur in a wide range of far-from-equilibrium systems including micro-mechanical oscillators, epidemiological and climate change models, and nonlinear electronic transport structures (e.g., doped semiconductor superlattices, tunnel diodes, and memristors). In the latter case, the phenomena are intimately connected to the presence of negative differential resistance (NDR), in which an increasing applied voltage causes a reduced electrical current, and bistability - the existence of two or more macroscopic current states for a given applied voltage. In this presentation, we discuss recent experimental measurements of noise-induced transition dynamics in a simple tunnel diode circuit driven by an analog broadband noise generator with variable intensity. We focus on the regime near the saddle node bifurcation that coincides with the end of bistability in the current-voltage curves. For sufficiently large noise intensity, we find that the logarithm of the mean switching time (from one to the other current state) scales as the 3/2 power of the distance to the bifurcation point and inversely with the noise intensity. Remarkably, this behavior holds over an unprecendentedly wide range of time scales. Thus, tunnel diode experimental data provide the most precise confirmation so far for longstanding theoretical predictions of scaling behavior of mean switching times near a saddle node bifurcation in a low-dimensional noise-driven nonlinear dynamical system.

Higher Order Dynamic Mode Decomposition

S. Le Clainche¹ and José M. Vega¹

¹School of Aerospace Engineering. Technical University of Madrid. Madrid, SPAIN

Standard dynamic mode decomposition (DMD) was introduced by Schmid (2010) using seminal ideas by Koopman (1931). This is a very useful method to post-process spatiotemporal data (resulting from generally nonlinear dynamics) as an expansion of spatial modes times exponentials in the time variable (to be called Fourier-like expansion), which exhibit generally nonzero growth rates. As such, DMD is an advantageous alternative to more classical methods to obtain such expansions (with zero growth rates), such as fast Fourier transform or power spectral density. However, standard DMD does not always give the correct results, even in cases in which the provided data admit an exact Fourier-like expansion. A recent method by the authors (2017), called higher order DMD (HODMD), solves this difficulty by essentially applying standard DMD to a set of enlarged snapshots that also contains time-delayed snapshots. Thus, HODMD synergically combines standard DMD and direct consequences of the well-known Takens' delay embedding theorem (1981). The new method will be illustrated using some toy-model dynamics and its performance will be tested using both, numerically generated databases from various nonlinear dynamical systems (complex Ginzburg-Landau equation, thermal convection in rotating spherical shells, cylinder wake) and experimental PIV measurements (zero-net-mass-flux jet and confined non-isothermal flows around vortex promoters). Some preliminary results on nuclear magnetic resonance data will also be presented.

Lossless Polariton Solitons

Stavros Komineas,¹ Stephen Shipman,² and Stephanos Venakides³

¹Department of Mathematics and Applied Mathematics, University of Crete, GREECE ²Department of Mathematics, Louisiana State University, USA ³Department of Mathematics, Duke University, USA

Photons and excitons in a semiconductor microcavity interact to form exciton-polariton condensates. These are governed by a nonlinear quantum-mechanical system involving exciton and photon wavefunctions. We calculate all non-traveling harmonic soliton solutions for the one-dimensional lossless system. We find two frequency bands of bright solitons when the inter-exciton interactions produce an attractive nonlinearity and two frequency bands of dark solitons when the nonlinearity is repulsive. In addition, there are two frequency bands for which the exciton wavefunction is discontinuous at its symmetry point. One of the bands of continuous dark solitons merges with a band of the discontinuous ones, forming a larger band. The far fields of the solitons in the lowest and highest frequency bands (one discontinuous and one continuous dark) are linearly unstable, whereas the other four bands, including the merged band of dark solitons, have linearly stable far fields. Poster session

Numerical simulation of the auto-rotation of a winged seed

<u>G. Arranz</u>,¹ M. Moriche,¹ O. Flores,¹ and M. García-Villalba¹

¹Bioeng. and Aerospace Eng. Department, Universidad Carlos III de Madrid, Leganés, SPAIN

Winged-seeds, or *samaras*, as they are usually called, are seeds from different tree species which start auto-rotating as they fall from the tree. Thanks to this auto-rotating motion, samaras are able to decrease their descend speed so as to take advantage of lateral wind gusts to disperse over large areas.

This phenomenon is produced due to the coupling between the inertia properties of the seeds and the aerodynamic forces. This makes the problem non-linear and very interesting to study. Moreover, recent research (Lentink *et al.*, 2009) showed the existence of a strong and stable vortex above the seeds as they auto-rotate. This kind of vortical structures are also present in the flapping flight of insects, birds and bats and are of interest for the development of small micro air-vehicles (MAV).

Therefore, we perform direct numerical simulations (DNS) to solve the Navier-Stokes equations coupled with the rigid-body equations of motion of a winged seed to study its auto-rotational flight. Apart from identifying the vortex that develops above the seed, we also investigate the effect that changing the Reynolds number has on the fluid and on the kinematics of the seed.

Optical properties of the dispersive *LiNbO*₃ nanoparticles composites

<u>R.M. de la Cruz</u>,¹ C. Kanyinda-Malu,¹ and J.E. Muñoz-Santiuste¹

¹Departamento de Física, Escuela Politécnica Superior, Universidad Carlos III de Madrid, Leganés, SPAIN

The silver (Ag)-embedded lithium niobate $(LiNbO_3)$ composites are theoretically analyzed under the effective medium Maxwell-Garnett approximation to account on the optimal conditions through which such composites present negative epsilon conditions. The dielectric function of Ag nanoparticles (NPs) is described by Drude theory with an additional Lorentz oscillator term to take into account the interband electronic transitions which typically occur in noble metals. The $LiNbO_3$ dielectric function is evaluated through the Sellmeier equations. Once the effective dielectric function (ϵ_{eff}) is evaluated, we investigate the negative epsilon condition ($\epsilon'_{eff} < 0$) as a function of the frequency. The results showed that, for given volume fraction values, the negative epsilon (NE) condition is satisfied for critical sizes of Ag NPs. This condition defines an interval of energies, called NE range. That NE range enlarges for increasing radius and becomes narrower for decreasing volume fractions. Furthermore, the calculated Fröhlich frequency is nearly close to the lower-energy limit of NE range. In addition, the calculated extinction spectra of the composite are analyzed in terms of the radius of Ag NPs.

Instability of laminar low-density jets

<u>D. Gómez-Lendínez</u>,¹ W. Coenen,¹ and A. Sevilla¹

¹Department of Thermal Engineering and Fluid Mechanics, Universidad Carlos III de Madrid, Leganés, SPAIN

The stability of laminar axisymmetric low-density jets has been investigated experimentally (Kyle & Sreenivasan 1993, Hallberg & Strykowski 2006) and with linear analysis (Coenen & Sevilla 2012, Coenen *et al.* 2017). In this work, Direct Numerical Simulations using FreeFEM++ (Hecht 2012) with P1 elements for pressure and P2 for velocity and density are performed to complement the abovementioned studies. Using the Stuart–Landau model to fit the numerical results for the self-excited oscillations we have computed a neutral stability curve that shows good agreement with experiments and stability theory.

Deformation of bacterial colonies growing on agar substrates

<u>S. Iakunin¹ and L.L. Bonilla¹</u>

¹Grupo de Modelización y Simulación Numérica, Universidad Carlos III de Madrid, Leganés, SPAIN

Some species of bacteria (like *Bacillus subtilis*) are famous for their ability to organize colonies (also called *biofilm*) into complex structures with folds and wrinkles. Emergent patterns contain a plenty of information about development of the colony and properties of the material, therefore studying these structures helps to understand better formation of biofilms what can be beneficial to control bacterial growth in industrial and medical applications. We simulate biofilm as a thin film deformed under effect of internal growth and bonded to a viscoelastic agar substrate. Deformation of thin plates can be described by Föppl-von Kármán equations which we modify by adding growth and substrate. Analysis of the model shows that wrinkles can appear as a result of growth incompatibility and their frequency increases due to interaction with the agar layer. Formulation of the problem in a weak form allows us to develop a numerical procedure based on finite element method and simulate deformations of biofilm for a wide spectrum of different growths.

An itinerant oscillator model with cage inertia for an intruder in granular liquid experiments

<u>Antonio Lasanta¹</u> and Andrea Puglisi²

¹G. Millan Institute, Fluid Dynamics, Nanoscience and Industrial Mathematics, Department of Materials Science and Engineering and Chemical Engineering, Universidad Carlos III de Madrid, Leganés, SPAIN ²CNR-ISC and Dipartimento di Fisica, Università La Sapienza, p.le A. Moro 2, 00185 Rome, ITALY

Recent experiments with a rotating probe immersed in weakly fuidized granular materials show a complex behavior on a wide range of timescales [1] (see fig 1). Viscous-like relaxation at high frequency is accompanied by an almost harmonic dynamical trapping at intermediate times, with possibly anomalous long time behavior in the form of superdiffusion. Inspired by the Itinerant Oscillator model for diffusion in molecular liquids, and other models with coupled thermostats acting at different timescales, here we discuss a new model able to account for fast viscous relaxation, dynamical trapping and super-diffusion at long times. The main difference with respect to liquids, is a non-negligible cage inertia for the surrounding (granular) fluid, which allows it to sustain a slow but persistent motion for long times. The computed velocity power density spectra and mean-squared displacement qualitatively reproduce the experimental findings. We also discuss the linear response to external perturbations and the tail of the distribution of persistency time, which is associated with superdiffusion, and whose cut-off is determined by cage inertia [2].

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The effect of surface viscosity on the capillary instability of liquid threads

<u>A. Martínez-Calvo¹</u> and A. Sevilla¹

¹Grupo de Mecánica de Fluidos, Universidad Carlos III de Madrid, Leganés, SPAIN

We study the capillary instability of a liquid thread in inviscid surroundings taking into account the effect of the surface viscosity by means of the Boussinesq–Scriven constitutive equation. We show that the problem is governed by four dimensionless parameters: the capillary Reynolds number, the elasticity parameter, the Boussinesq number, and the ratio of the shear and dilatational surface viscosities. Finally, we provide a systematic study of the maximum growth rate and the corresponding wavenumber in a wide region of parameter space.

Nonlinear resonance in a combined elastic solid-granular structure

Aurélien Merkel,¹ G. Theocharis, F. Allein, J.-P Groby, V. Tournat, and V. Gusev

¹Insituto Gregorio Millan Barnaby, Universidad Carlos III de Madrid, 28916 Leganés, Madrid, SPAIN

In this study, longitudinal elastic waves are excited within a cylindrical solid rod, which is in contact at one extremity with an elastic bead. The diameter of the rod is small compared to the wavelength, the wave propagation is considered as one-dimensional. Moreover, the wave propagation in the rod is considered as linear. The sphere-plane contact shows a highly nonlinear behavior as expected from the Hertz's model of contact. The contact is modeled by a nonlinear spring and the bead by a rigid mass, the mass-spring system is then considered as nonlinear isolated resonator.

The resonance curves of the nonlinear mass-spring system depend on the excitation amplitude, where a downshift of the resonance frequency with increasing excitation amplitude is observed. The prediction of the resonance frequency shift by the Hertz's model is compared to the experimental results and shows a disagreement. A better agreement is found by considering the visco-elastic losses with a viscoelastic model of contact between a sphere and a plane, namely the Kuwabara and Kono or Brilliantov model.

The observation of the nonlinear effects linked to the resonance of the mass-spring system can lead to the design of nonlinear elastic metamaterials, where the wave propagation is controlled by nonlinear isolated resonators.

Chaos generation in a semiconductor superlattice coupled to a linear resonator at room temperature

Emanuel Mompó,¹ Manuel Carretero,¹ and Luis L. Bonilla¹

¹Grupo de Modelización, Simulación Numérica y Matemática Industrial, Universidad Carlos III de Madrid, Leganés, SPAIN

Random Bit Generators (RBG) are of great technological interest, since they are fundamental for data security through encryption, stochastic modeling, Monte-Carlo simulations, even online gambling games.

Classical generators can be either insecure or slow. Recent solutions that avoid these kind of problems include semiconductor superlattices, which can produce spontaneous chaotic oscillations at room temperature. Theoretical study of these aspects of electron transport in superlattices is recent and needs to be completed.

In this work we studied the dynamics that take place when a superlattice is coupled to a monochromatic resonator at room temperature. That is, if the mere presence of a superlattice allows the resonator to (strongly) embrace a chaotic behaviour.

Thermoelectricity without absorbing energy from the heat sources

<u>R. Sánchez</u>,¹ R. Whitney, F. Haupt, and J. Splettstoesser

¹Grupo de Modelización, Simulación Numérica y Matemática Industrial, Universidad Carlos III de Madrid, Avda. de la Universidad 30, 28911 Leganés, SPAIN

A thermocouple generates finite electrical power by coupling a part of an electrical conductor to an external heat source. Macroscopically, this part of the system equilibrates to an increased temperature that governs the thermoelectric performance. The generated power then depends on the heat current absorbed from the source. In a mesoscopic system, this is not necessarily the case. The coupling of a nanoscale system (e.g. a quantum dot) to a hot and a cold bath can be used to generate a finite power in the electrical conductor even in situations when it absorbed no heat. We show that this effect is possible in the presence of non-thermalized states [1]. We propose a configuration based on capacitively coupled quantum dots recently realized experimentally [2, 3], but the effect does not rely on the presence of interactions.

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A soliton drives tumor-induced angiogenesis

F. Terragni,¹ M. Carretero,¹ and L.L. Bonilla¹

¹Grupo de Modelización, Simulación Numérica y Matemática Industrial, Universidad Carlos III de Madrid, Avda. de la Universidad 30, 28911 Leganés, SPAIN

Angiogenesis is a complex multiscale process in which blood vessels are generated and grow in a living tissue. Although a physiological process, which is essential for organ development and repair, unbalanced angiogenesis can lead to various disorders.

Hypoxic tumoral cells produce vessel endothelial growth factors that stimulate the creation of new capillary sprouts and the proliferation of the vessel network, through which needed oxygen and nutrients are thus transported to the tumor.

A hybrid mesoscale tip cell model (in which vessel tips trajectories are the capillaries advancing towards the tumor) is described. Vessels elongation and sprouts movement by chemotaxis (i.e. via gradients of growth factors) are modeled by stochastic equations coupled to reaction-diffusion equations for the concentration of involved substances. Branching of new tips and anastomosis (namely, the destruction of tips that merge with existing vessels) are also taken into account.

It is shown that a deterministic description can be found for the density of active vessel tips obtained by ensemble averages over many replicas of the stochastic process. More interestingly, such density forms a stable soliton-like wave whose location, velocity and size can be characterized by a system of collective coordinates ODEs. Integrating the latter allows to simplify the control task of predicting the average time-evolution of the angiogenic tip density from a primary vessel to the tumor.

Collective cell motion in epithelial surfaces

 $\underline{\operatorname{Carolina}\,\operatorname{Trenado}},^1$ Javier $\operatorname{Rodríguez},^2$ and Luis L. Bonilla^1

¹Grupo de Modelización y Simulación Numérica, Universidad Carlos III de Madrid, Leganés, SPAIN ²Universidad Carlos III de Madrid, Leganés, SPAIN

Collective migration of epithelial cells plays an important role in tissue growth and wound healing. One of the many interesting aspects of particle systems is its behaviour during the phase transition which is analyzed through the concept of order parameter. For this reason, we studied the displacement of cells moving in a collective way by means of numerical simulations and theoretical analysis of biological processes. In particular, the model is based on two assumptions, namely, the cells move in an stochastic way and also adapt their motion to that of their nearest neighbors. In addition, we reproduced (with a modified model) the behaviour of the system moving in an epithelium border.

Cellular dynamics model of angiogenesis

Rocío Vega,
1 Manuel Carretero,
1 and Luis L. Bonilla
1 $\,$

¹Grupo de Modelización, Simulación Numérica y Matemática Industrial, Universidad Carlos III de Madrid, Avda. de la Universidad 30, 28911 Leganés, SPAIN

Angiogenesis, the formation of new blood vessels from existing vasculature, is the basis of organ growth and repair in healthy conditions and of pathological developments such as cancerous tumors. Angiogenesis is a multiscale process, ranging from gene transcription and protein synthesis, through the cell dynamics and right up to the level of organization of tissues and organs.

In this poster, we present a cell-based model structured in terms of these multiple scales by incorporating extracellular and cellular levels as well as the results of simulations. At extracellular level, the model considers chemotaxis and durotaxis by adding an equation for the Vascular Endothelial Growth Factor and Finite Element computational model for the compliant extracellular matrix, respectively. At the cellular level, a cellular Potts model considers cell migration, growth, proliferation, cellular adhesion, distinction between tip and stalk phenotypes, sprout branching and anastomosis. The extracellular and cellular level are coupled giving rise to a model that incorporates biomechanical and biochemical mechanisms allowing to simulate branching based on purely biological properties.