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**SEGUNDO ENCUENTRO DE LA RED
DE FÍSICA DE SISTEMAS FUERA
DEL EQUILIBRIO**

Leganés

20-22 de enero de 2010

Miércoles 20 de enero

09:30-09:45 Presentación

09:45-10:30 Guy Joulin

Potential-flow models for 2D premixed flames, and beyond

10:30-11:00 Pedro Luis García-Ybarra

PIV measurements of the local burning velocity in laminar Bunsen flames of methane-air mixtures

11:00-11:30 Café

11:30-12:15 Amable Liñán

Initiation of reactive fronts by heat deposition with external energy sources

12:15-12:45 Santiago Madruga

Stability and structure in films of binary mixtures with free surfaces

12:45-13:15 Ignacio Pagonabarraga

Inestabilidades de mojado en frentes líquidos capilares forzados

13:15-13:35 Wilfried Coenen

Viscous stability analysis of parallel flows with discontinuous base profiles

13:35-15:00 Comida

15:00-15:30 Andrés Santos

Free cooling of a binary granular fluid of inelastic rough hard spheres

15:30-16:00 Antonio Astillero

Estudio del comportamiento hidrodinámico no newtoniano en gases granulares mediante simulaciones directas de Monte Carlo y computación grid

16:00-16:30 Café

16:30-17:00 José María Ortiz de Zárate

Ilustración del teorema de Jarzynski con sistemas sencillos

17:00-17:30 Enrique Abad

Derivación mesoscópica de ecuaciones fraccionales de subdifusión y de subdifusion-reacción y aplicación a problemas de búsqueda de un “target”

Jueves 21 de enero

10:00-10:30 Christian Ertler

Magnetolectric feedback effects in magnetic resonant tunneling structures

10:30-11:00 Sigmund Kohler

Current noise in ac-driven mesoscopic conductors

11:00-11:30 Café

11:30-12:00 Eugene Ya. Sherman

Optical injection and evolution of charge and spin currents in quantum wells

12:00-12:30 David Sánchez

Magnetoasymmetries and nonlinear fluctuation relations in mesoscopic conductors

12:30-13:00 Manuel Carretero

Phase diagrams and switching of voltage and magnetic field in diluted magnetic semiconductor nanostructures

13:00-13:30 Anders Mathias Lunde

Interaction induced edge channel equilibration

13:30-15:00 Comida

15:00-15:30 Javier Rodriguez-Rodriguez

The locomotion of terrestrial gastropods: Can a snail crawl on a Newtonian fluid?

15:30-16:00 Javier Burguete

Inestabilidades de fluidos conductores en cavidades cilíndricas

16:00-16:30 Café

16:30-17:00 Susana Serna

Propagación de frentes con velocidad función no lineal de la señal

17:00-17:20 Paolo Malgaretti

Collective effects in intracellular transport

Viernes 22 de enero

9:45-10:30 David G. Schaeffer

Chaotic behavior in a one-dimensional cardiac model

10:30-11:00 Blas Echebarria

Modelling cardiac dynamics: What can we learn from simple models?

11:00-11:30 Café

11:30-12:15 Bjorn Birnir

A simulation of the life-cycle of myxobacteria

12:15-12:45 Juan Diego Álvarez

Recovering the geometrical properties of a cardiac ischemia: An inverse problem approach

12:45-13:15 Rosa López

Competition between Kondo effect and reservoir-mediated superexchange in double quantum dots

13:15-13:45 José M. Vega

Accelerating numerical solvers using POD+Galerkin projection

13:45-15:00 Comida

Potential-flow models for 2D premixed flames, and beyond

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The dynamics of two-dimensional thin premixed flames is addressed in the framework of mathematical models where the flow field on either sides of the front is piecewise incompressible and vorticity-free. Flames confined in channels with asymptotically-straight impenetrable walls are considered. Beside a few free propagations along straight channels, we focus on flames propagating against high-speed flows and anchored at a round central obstacle, or at two symmetric bumps protruding inward. Combining conformal maps and Green's functions, a regularised generalisation of Frankel's integro-differential equation for the instantaneous front shape is derived in each configuration, and solved numerically. This produces a wealth of real-looking phenomena: steady fronts, symmetric or not, noise-induced sub-wrinkles and fuzzy flash-back events. Open mathematical/physical problems and perspectives are evoked. In particular, we sketch how recent works can 'potentially' extend all this to even more general channels while retaining the effects of combustion-generated vorticity.

PIV measurements of the local burning velocity in laminar Bunsen flames of methane-air mixtures

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Bunsen flame is a classical example of an axisymmetric concave flame configuration where the increase of local burning velocity by flame compression (negative stretch) is shown, noticeably at the flame tip. At any point the flame is curved and strained, and each effect contributes separately to the strain rate of the flame area which changes the local burning velocity with respect to the burning velocity of a planar flame. By assuming that both contributions are linear, the reactive mixture is characterized by the two proportionality factors, which are known as Markstein lengths. In quasi planar configurations, the Markstein lengths are equal and the two effects add up into a single term: the so-called flame stretch. Markstein lengths can be determined experimentally by simultaneously measuring the curvature of the flame, the strain rate of the flow and the local burning velocity of the flame. To achieve this goal, we have set up a laminar jet burner and used a PIV system to measure the gas flow velocity in the vertical cross-section through the axis of methane - air Bunsen flames. The PIV system is composed by a double Nd:YAG pulse laser (New Wave 120XT) with a sheet forming emission optics, a double-shuttered camera (PCO, 13921040 pixels) and a pulse generator (ILA). To track the flow, the air is seeded with oil droplets formed by evaporation - condensation in a seeding chamber inserted in the air line. The laser sheet allows the visualization of the oil droplets before they evaporate in the flame preheating region, which permits the determination of the upstream gas flow velocity with the ViDPIV cross-correlation software. Even more, the long exposure picture of each PIV couple allows to receive enough flame radiation, in the laser wavelength that goes through the filter of the camera, to visualize the reactive front position and measure the local front curvature.

Initiation of reactive fronts by heat deposition with external energy sources

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A mixture of fuel and air may sustain in general two different types of reactive fronts called deflagrations –very subsonic and diffusion controlled– and detonations –markedly supersonic and with an inviscid ZND structure including a strong leading shock wave. The occurrence of one or the other depends on the intensity of the initiation process. We shall begin by describing in the absence of chemical reactions the temperature and flow fields associated with concentrated sources of heat. Afterwards, we shall show how this analysis provides the initial conditions allowing us to calculate, in the reactive case, the minimum energy for the successful initiation of deflagrations. We shall also give a brief description of the corresponding initiation of detonations.

Stability and structure in films of binary mixtures with free surfaces

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Thin polymer films are often used in advanced technological applications either as homogeneous coatings or as structured functional layers. Their stability and potential use is mostly determined by the wettability properties of the substrate and is well understood for single component liquids. However, in many relevant applications the film consists of a binary mixture such as a polymer blend. For such systems the dynamics of the decomposition within the film and of the dewetting of the film itself may couple. This allows for new pathways of structuring like decomposition induced dewetting.

We present a model for thin films of binary mixtures, such as polymer blends, with free surfaces that allows the study of the coupling between profile evolution and decomposition. The model is based on model-H [1] describing the coupled transport of concentration (convective Cahn-Hilliard equation) and momentum (Navier-Stokes-Korteweg equations) fields supplemented by boundary conditions at the substrate and the free surface.

After determining homogeneous and vertically stratified base states of free surface films of polymer mixtures we analyse their linear stability with respect to lateral perturbations [2]. For purely diffusive transport, an increase in film thickness either exponentially decreases the lateral instability or entirely stabilizes the film. The inclusion of convective transport leads to a further destabilization as compared to the purely diffusive case. In some cases the inclusion of convective transport and the related widening of the range of available film configurations (it is then able to change its surface profile) change the stability behavior qualitatively [3].

We furthermore present results regarding the dependence of the instability on several other parameters, namely, the Reynolds number, the Surface tension number and the ratio of the typical velocities of convective and diffusive transport.

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[2] U. Thiele, S. Madruga, and L. Frastia. *Phys. of Fluids.* **19**, 122106 (2007).
[3] S. Madruga and U. Thiele. *Phys. of Fluids*, **21**, 062104 (2009).

Inestabilidades de mojado en frentes líquidos capilares forzados

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En esta charla analizaré las posibilidades de explotar las propiedades de mojado del sustrato sobre el que se mueve un frente fluido capilar para controlar las morfologías del frente. En particular, discutiré resultados obtenidos por simulación numérica de la capacidad de usar sustratos con propiedades heterogéneas que modulan su hidrofobicidad para promover el desarrollo de dedos y la posible emisión de gotas así como sus potenciales aplicaciones en microfluídica.

Viscous stability analysis of parallel flows with discontinuous base profiles

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The viscous linear instability of parallel shear flows with piecewise constant base profiles is considered in the limit of low Mach numbers, both for planar and axisymmetric geometries such as mixing layers, jets and wakes. Our results generalize those of Drazin (*J. Fluid Mech.* vol. 10, 1961, p. 571), by contemplating the possibility of arbitrary jumps in density and transport properties between two uniform streams separated by a vortex sheet. The eigenfunctions, obtained analytically in the regions of uniform flow, are matched through an appropriate set of jump conditions at the discontinuity of the basic flow, derived here by repeated integration of the linearized conservation equations in their primitive variable form. The validity of the resulting algebraic dispersion relation, given here in closed form, is assessed with the aid of numerical calculations performed with continuous profiles and is applied, in particular, to study the effects of molecular diffusivity on the spatiotemporal stability of parallel inhomogeneous jets and wakes with very thin shear layers.

Free cooling of a binary granular fluid of inelastic rough hard spheres

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The simplest model of a granular fluid consists of a system of identical, inelastic smooth hard spheres with a constant coefficient of normal restitution. Obviously, the model can be made closer to reality by introducing extra ingredients. In particular, polydispersity and roughness are especially relevant because they unveil an inherent breakdown of energy equipartition in granular fluids, even in homogeneous and isotropic states. In this work a fluid mixture of inelastic rough hard spheres of arbitrary number densities, masses, diameters, moments of inertia, and mutual coefficients of normal and tangential restitution is considered. First, the collisional energy production rates associated with the translational and rotational temperatures are derived by kinetic-theory arguments. Next, the results are applied to the homogeneous free cooling of a binary mixture and the steady values of the three independent temperature ratios are analyzed. Finally, the time evolution of those ratios is investigated to understand the origin of a paradox in the quasi-smooth limit.

Estudio del comportamiento hidrodinámico no newtoniano en gases granulares mediante simulaciones directas de Monte Carlo y computación grid

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Un gas granular no exhibe nunca un estado de equilibrio debido a que tiene lugar una disipación continua de energía como consecuencia del carácter inelástico de las colisiones entre las partículas que lo constituyen. Debido a esto, la posibilidad de utilizar una descripción de tipo hidrodinámico para esta clase de sistemas físicos no es del todo obvia [1]. Tal descripción, de existir, no debería limitarse exclusivamente a las ecuaciones de Navier–Stokes, si no que debería incluir todos aquellos estados donde la dependencia espacial y temporal de la función de distribución de velocidades $f(\mathbf{r}, \mathbf{v}, t)$ venga dada por una dependencia funcional de los campos hidrodinámicos $n(\mathbf{r}, t)$, $\mathbf{u}(\mathbf{r}, t)$ y $T(\mathbf{r}, t)$. Dicho de otro modo, $f(\mathbf{r}, \mathbf{v}, t) = f[\mathbf{v}|n, \mathbf{u}, T]$.

Teniendo presente lo dicho en el párrafo precedente, dado cualquier estado inicial, la evolución del mismo sucederá en dos etapas consecutivas. Inicialmente, el gas granular experimentará una etapa *cinética* breve (de unas pocas colisiones por partícula de duración) y que además depende en gran medida de las condiciones iniciales. A continuación seguirá una etapa *hidrodinámica* más lenta donde la influencia de las condiciones iniciales prácticamente ha desaparecido. Por último y en el caso de existir una fuente externa de energía que compense la disipación inelástica debida a las colisiones, el gas alcanzará un estado estacionario de no equilibrio.

Uno de los objetivos principales de este trabajo ha sido analizar la susodicha etapa hidrodinámica. Para acometer esta tarea, hemos considerado un gas granular monocomponente y hemos efectuado simulaciones directas de Monte Carlo DSMC [4] en un entorno basado en computación grid [5]. También hemos considerado dos estados diferentes y paradigmáticos de no equilibrio. El primero de ellos ha sido el flujo tangencial uniforme (USF) [2]. Este flujo se caracteriza por una densidad constante n , una temperatura granular $T(t)$ dependiente del tiempo (pero uniforme) y un campo de velocidades de la forma $\mathbf{u}(\mathbf{r}) = ay\hat{\mathbf{x}}$, donde a es el gradiente de velocidad (el valor de a es constante). El segundo de los flujos considerados ha sido el flujo longitudinal uniforme (ULF) [3]. Las características básicas de este flujo son un campo de velocidades longitudinal y lineal $u_x(x, t) = a(t)x$, donde $a(t) = a_0/(1 + a_0t)$ es el gradiente de velocidad, una densidad uniforme $n(t) \propto a(t)$ y una temperatura granular $T(t)$ también uniforme. En un gas granular caracterizado por un coeficiente de restitución normal constante α , el parámetro de control relevante del problema es el gradiente de velocidad reducido $a^* = a(t)/\nu(t)$ (que representa el papel de número de Knudsen), donde $\nu(t) \propto n(t)\sqrt{T(t)}$ es una frecuencia de colisión efectiva. El parámetro de respuesta relevante es la viscosidad tangencial no lineal $\eta^*(a^*)$ definida a partir de la diferencia entre la tensión normal $P_{xx}(t)$ y la presión hidrostática $p(t) = n(t)T(t)$.

Hemos comparado los resultados de las simulaciones con los proporcionados por modelos cinéticos simplificados mostrando un acuerdo muy bueno. Por ejemplo, en el caso particular del flujo longitudinal uniforme, la comparación de los resultados correspondientes a la viscosidad tangencial no lineal $\eta^*(a^*)$ obtenidos mediante un modelo cinético tipo BGK y a

través de las simulaciones, muestra un acuerdo excelente tanto para el punto correspondiente al estado estacionario como a la totalidad de la función no newtoniana $\eta^*(a^*)$.

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- [2] A. Astillero and A. Santos, Europhys. Lett. **78**, 24002 (2007).
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Ilustración del teorema de Jarzynski con sistemas sencillos

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En mi presentación ilustraré el teorema de Jarzynski considerando dos ejemplos sencillos de sistemas ideales, en los que el cálculo del trabajo irreversible puede hacerse de forma explícita y analítica. En particular repasaré publicaciones de otros autores referidos a un gas ideal unidimensional y presentaré resultados para un sistema de dos paredes unidas por osciladores armónicos (muelles). A partir del análisis de estos sistemas sencillos se puede conseguir una mejor comprensión de la relevancia del resultado de Chris Jarzynski.

Derivación mesoscópica de ecuaciones fraccionales de subdifusión y de subdifusión-reacción y aplicación a problemas de búsqueda de un “target”

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El estudio de sistemas cuyos constituyentes satisfacen leyes no markovianas de evolución adquiere en la actualidad especial relevancia a la luz de recientes experimentos que ponen de manifiesto la importancia de efectos de memoria en una larga serie de sistemas físicos, químicos y biológicos. En sistemas donde el transporte mediante saltos aleatorios juega un papel central, es bien sabido que los efectos de memoria pueden describirse empleando ecuaciones maestras generalizadas que contienen distribuciones de cola larga. Un caso particular pero paradigmático es la ecuación integral para el CTRW (continuous time random walk), aplicada con éxito a multitud de problemas (transporte de excitaciones en sólidos amorfos, procesos de envejecimiento, evolución de mercados financieros, etc.). Para una distribución apropiada de tiempos de espera, la cinética engendrada por el CTRW en escalas de tiempo suficientemente largas se puede captar mediante una ecuación fraccional de subdifusión (EFS). La EFS es una ecuación que se caracteriza por la presencia de un operador integrodiferencial denominado derivada fraccional de Riemann-Liouville. El desplazamiento cuadrático medio de las partículas cuyo movimiento describe la EFS crece como t^γ , donde $0 < \gamma < 1$.

Empezaremos nuestra presentación con un breve recordatorio de la derivación de la EFS a partir de la ecuación integral del CTRW. Tomando la derivación de la EFS como punto de partida, mostraremos cómo llegar a una (nueva) ecuación fraccional de subdifusión-reacción (EFSR) introduciendo un término reactivo a nivel del CTRW.

En segunda instancia, pasaremos a estudiar una aplicación concreta de la EFS y la EFSR. Se trata del cálculo de la probabilidad de supervivencia $P(t)$ de una partícula o “target” rodeada por un medio poblado por trampas subdifusivas. Este tipo de problemas de búsqueda de un target juega un papel especialmente relevante en un contexto biológico. Imaginemos por ejemplo que unos ligandos (=trampas) distribuidos aleatoriamente en el medio intracelular buscan una proteína (=target) para asociarse a ella y que el tiempo necesitado para la unión es mucho menor que el tiempo típico de difusión en el medio celular. Supongamos además que los tiempos de espera entre pequeños saltos consecutivos de los ligandos en el medio intracelular siguen una distribución de probabilidad de cola larga y que el CTRW subyacente da un movimiento subdifusivo en escalas de tiempo suficientemente grandes. Entonces una descripción en términos de una EFS resulta pertinente y $P(t)$ puede identificarse como la probabilidad de que la unión entre la proteína y cualesquiera de los ligandos *no* se haya producido después de un tiempo t . Estudiaremos el comportamiento de $P(t)$ para tiempos largos cuando el target no se mueve, cuando su movimiento es subdifusivo, y cuando es difusivo normal. Si además admitimos la posibilidad de que los ligandos se degraden espontáneamente en el curso de su movimiento subdifusivo, entonces la cinética de los mismos no vendrá dada por la EFS, sino por la EFSR. Aquí estudiamos también $P(t)$, aunque limitándonos al caso de un target inmóvil. Concluimos que el comportamiento de $P(t)$ es extremadamente sensible al tipo de movimiento del target y a la velocidad de degradación de las trampas.

Magnetoelectric feedback effects in magnetic resonant tunneling structures

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The development of ferromagnetic dilute magnetic semiconductors (DMSs) with reasonably high Curie temperatures such as GaMnAs has strongly stimulated the survey of designing all-semiconductor spintronic devices. Especially, heterostructures made of stacked layers of both magnetic and nonmagnetic semiconductors provide a lot of opportunities for controlling and tuning their spin-dependent transport properties. For instance, highly efficient spin valves, spin switching and spin filtering devices have been demonstrated by exploiting magnetic resonant tunneling structures [1].

Here, we show that in resonant tunneling structures, which comprise a ferromagnetic quantum wells made of a DMS-material, interesting dynamical effects can occur [2]. In such systems the transport and magnetic properties become strongly coupled, since the ferromagnetic order in the quantum well is mediated by the itinerant carriers, which can tunnel in and out of the well. Both the Coulomb interaction of the particles and the magnetic exchange field, which causes a spin splitting of the well subbands, give rise to strong feedback effects on the tunneling current. Interestingly, for a broad voltage range self-sustained high-frequency oscillating currents associated with an oscillating well magnetization appear. The requirements for the occurrence of these dc-driven magnetoelectric oscillations are investigated and possible device setups, which should allow for an experimental observation, are discussed.

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Current noise in ac-driven mesoscopic conductors

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Electromagnetic ac fields can alter significantly the transport properties of mesoscopic systems such as molecular wires and coherently coupled quantum dots. Resonant excitations of electrons, e.g., enhance drastically the time-averaged currents. These systems may also be used to study the so-called ratchet or pump effect: in asymmetric conductors, an ac field induces a dc current even in the absence of any bias voltage. In the presence of a magnetic field, spin pumping is possible as well. The interplay between the driving and a static disorder may support or suppress pumping.

The corresponding transport mechanisms leave their fingerprints also in the noise whose relative strength characterized by the Fano factor. In general, we find that resonant excitations reduce the noise level while current suppressions are accompanied by a noise reduction.

In our studies, we model the external field by a periodic time-dependence of the wire Hamiltonian. This requires a generalization of established transport theories like, e.g., the Landauer formula or master equation approaches. We present such a generalization that is based on the Floquet theorem. It allows one to compute the full nonlinear response to the driving field, which in some cases is essential.

Optical injection and evolution of charge and spin currents in quantum wells

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We consider optically injected charge and spin currents in semiconductor quantum wells. The injection can be done by quantum optics techniques with interference of one- and two-photon transition processes, by intersubband light absorption, and by a stimulated Raman process. The final state currents strongly depend on the injection process, producing the system very strongly out of the equilibrium for the interband transitions and relatively weakly out of the equilibrium for the Raman process. In addition to the directly excited, the spin currents can arise due to the spin-dependent scattering of electrons by charged impurities.

Next, we consider relaxation of injected currents, where the system symmetry is initially broken. The subsequent nonequilibrium dynamics is governed by the spatially varying long-range Coulomb forces, disorder, and electron-hole collisions. As a result, inhomogeneities in the charge and velocity distributions should develop rapidly and lead to previously unexpected consequences for the experiment. We suggest that the system eventually evolves into a behavior similar to chaos.

Magnetoasymmetries and nonlinear fluctuation relations in mesoscopic conductors

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In the nonlinear regime of electron transport, screening effects can lead to a breakdown of microreversibility in mesoscopic systems. The nonequilibrium response of the potential landscape along the system is, quite generally, an uneven function of the magnetic field, implying a magnetoasymmetry of the differential conductance [1]. This effect has been observed in many different phase-coherent conductors [2]. Recent theoretical developments relate the asymmetry of the noise to the asymmetry of the differential conductance in the leading order of a voltage expansion [3, 4]. As a consequence, a higher-order fluctuation dissipation relation (FDR) is established between the two magnetoasymmetries even when fluctuation theorems are not obeyed. Here, we discuss the magnetoasymmetries arising in the current fluctuations of quantum dots with strong Coulomb correlations and explicitly demonstrate the validity of nonlinear FDRs when interactions are treated beyond the mean field approximation [5].

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Phase diagrams and switching of voltage and magnetic field in diluted magnetic semiconductor nanostructures

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We investigate the response of a n-doped dc voltage biased II-VI multi-quantum well diluted magnetic semiconductor nanostructure having its first well doped with magnetic impurities (Mn) under both voltage and magnetic-field abrupt switching. Transitions between stationary states and self-sustained current oscillations are systematically analyzed, obtaining the phase diagram of voltage versus level splitting induced by an external magnetic field. The phase diagram shows regions of stable self-sustained current oscillations immersed in a region of stable stationary states. Sudden voltage or magnetic field changes may switch or disconnect current oscillations from an initial stationary state, and reciprocally, current oscillations may disappear after sudden changes of voltage or magnetic field changes into the stable stationary states region. Our results show how to design a device operating as a spin injector and a spin oscillator by tuning the Zeeman splitting (through the applied external magnetic field and the density of magnetic impurities) and the parameters determining the sample configuration (number of wells, doping density, barrier and well widths, ...).

Interaction induced edge channel equilibration

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Two decades ago, edge states in integer quantum hall systems [1] were demonstrated to be a physical reality by creating a non-equilibrium population [2] through selective injection and detection of carriers in different states along the same edge [3–5]. Now in a series of novel experiments the group of Pierre [6, 7] has investigated the non-equilibrium distribution function in an edge state as it evolves along a channel away from a quantum point contact at which it is initially created. In this work, we calculate the electronic distribution functions of two Coulomb coupled chiral edge states. They form a quasi-1D system with broken translation invariance and the distribution function is found using the equation of motion approach. We find that relaxation and thereby energy exchange between the two edge states is determined by the shot noise of the edge states generated at a quantum point contact. In close vicinity to the quantum point contact, we derive analytic expressions for the distribution functions. We further give an iterative procedure with which we can compute numerically the distribution functions arbitrarily far away from the quantum point contact. Our results are compared with the recent experiments [6, 7].

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The locomotion of terrestrial gastropods: Can a snail crawl on a Newtonian fluid?

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The locomotion of terrestrial gastropods is driven by a train of periodic muscle contractions (waves) and relaxations (interwaves) that propagate from their tail to their head. We studied the locomotion of these animals on smooth flat surfaces by measuring their velocity, the frequency and wavelength of the pedal waves, and the traction forces they transmit to the substrate. In all cases studied, the surface of the ventral foot is lifted with the passage of each pedal wave and pressed to the substrate at the interwaves. Our measurements showed that a net forward traction force is indeed generated beneath each stationary interwave. Furthermore, a simple model based on lubrication theory is proposed. Unlike other models previously reported in the literature, ours explains the ability of the animal to crawl at a constant speed without requiring any special rheological property of the mucus.

Inestabilidades de fluidos conductores en cavidades cilíndricas

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Los flujos inducidos en fluidos conductores pueden ser radicalmente diferentes de los que se obtienen en condiciones análogas con fluidos no conductores. Una de las razones es la interacción con campos magnéticos, ya sean internos (autoinducidos) o externos (forzado). En este trabajo presentamos dos dispositivos experimentales que analizan estos problemas en cavidades cilíndricas.

En el primer caso se analizan las inestabilidades hidrodinámicas y magnetohidrodinámicas que aparecen en un flujo capaz de generar el efecto dinamo (autoexcitación de un campo magnético, mecanismo en el origen de los campos astrofísicos). Especial énfasis se hace en la bifurcación del flujo medio turbulento y la dinámica de estructuras coherentes (vórtices).

En el segundo caso, se presenta un experimento donde se fuerza una cavidad cilíndrica llena de un metal líquido con un campo axial dependiente del tiempo.

Propagación de frentes con velocidad función no lineal de la señal

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Consideramos una clase de ecuaciones de Hamilton-Jacobi que representan la propagación de frentes cuya velocidad es una función no lineal de la señal. Estas ecuaciones contienen un Hamiltoniano no estándar que permite la presencia de ondas de choque en su solución que se propagan con velocidad no lineal. Las ondas de choque se pueden formar en tiempo finito a partir de datos iniciales continuos. Esta nueva clase de ecuaciones de Hamilton-Jacobi se puede considerar una extensión de la teoría clásica de Crandall and Lions (1983) en la que las ecuaciones de Hamilton-Jacobi únicamente admiten soluciones viscosas continuas. Analizamos la estructura de la solución de la nueva clase de ecuaciones y proponemos un esquema numérico en diferencias finitas que captura los frentes de propagación con velocidad correcta. Presentamos una serie de ejemplos significativos de este tipo de ecuaciones como son la ecuación de Hamilton-Jacobi relativista y la ecuación de Hamilton-Jacobi de medios porosos.

Collective effects in intracellular transport

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Eukaryotic cells present a very complex network of “highways” on which materials like vesicles or organelles are actively transported. The carriers are molecular motors that produce mechanical work by the hydrolyzation of ATP. Each motor has a specific molecular structure that determines its mechanical properties like the velocity or the direction in which it walks along the biofilament. Moreover molecular motors exhibit rich dynamics: motors attach or detach from the biofilaments, motors that walk in the same direction can cooperate in the transport of the same cargo [1] while motors that walk in different directions can play a “tug of war” [2] when attached at the same cargo. Many models have been proposed to study molecular motors at different scales ranging from mechanochemical models for a single motor [3] to continuum models which describe large motor ensembles walking on the same track [4, 5].

We have modeled the molecular motors like Brownian motors that walk in a high viscous fluid. In particular, we are interested in the study of the hydrodynamic interactions between ensembles of motors walking on the same track. To study such interactions, we have developed a numerical model that permits us to couple the ratchet-like movement of motors to the cytoplasmic fluid they move in.

We have studied the velocities of ensembles of motors as a function of the concentration of motors, the fluid viscosity and the ratio between the dimension of the motor and the ratchet period. In all cases we have found a marked dependence of the motors’ average velocity on their concentration. We have assessed the relative relevance of direct motor-motor interaction and dynamical coupling through the solvent in the collective perspective of motor transport.

As a first result, we have found that for low concentration of motors the hydrodynamic coupling speeds up the motors while for high concentration values the excluded volume interaction between motors dominates and prevents motors to move in agreement with previous results on a simplified discrete 2D model [8]. In particular, while rising the motors’ concentration, we find that motors move in a coordinate way that speeds motors ensembles velocity up to 50 times the speed of a single motor. Moreover we noticed the formation of big clusters whose size scales with motors number. A preliminary analysis shows that their formation is strongly affected by the constraint imposed on motors trajectories on the biofilament (1D or 2D). Surprisingly the velocity of these structures, that are stable for long times compared with typical time scales of a single motor, is lower than the velocity we measured before clustering for the same motors’ concentration.

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Chaotic behavior in a one-dimensional cardiac model

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In electrocardiology, the term action potential refers to the behavior that, in response to a brief stimulus, the electrical potential across cardiac cell walls is elevated for an extended period. The duration of action potentials under periodic pacing is an important quantity clinically, physiologically, and mathematically. At slow to moderate pacing rates, every stimulus produces an action potential of the same duration, but at high pacing rates cardiac tissue often undergoes a bifurcation to what is called alternans: i.e., uniform APDs are replaced by an alternation between short and long action potentials. In a single cell or a small piece of cardiac tissue, this bifurcation is a familiar period-doubling bifurcation, but when propagation effects are important the nature of the bifurcation to alternans is far from clear. For example, the short/long alternation may suffer phase reversals at various locations in the tissue. This behavior, known as discordant alternans, is considered to be a precursor to ventricular fibrillation. In collaboration with my student, Shu Dai, I have studied these phenomena through an approximate equation (derived by Echebarria-Karma) for the modulation of nonuniform wave trains in one spatial dimension. In this lecture, after describing the context of the problem, I will report on this work. In particular, we have shown that: The modulation equation undergoes both Hopf and steady-state bifurcations; which bifurcation occurs first depends on a parameter derived from the speed of traveling waves; the competition between the two modes gives rise to interesting secondary bifurcation. Moreover, in certain parameter ranges, solutions of this equation exhibit chaotic behavior, as indicated in my title. While chaos has been observed in simulations of spiral waves in several dimensions, it is surprising to find it in a one-dimensional model.

Modelling cardiac dynamics: What can we learn from simple models?

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In cardiac muscle, a change in transmembrane cellular potential produces a response known as action potential, that propagates along tissue. Many cardiac malfunctions are associated to problems in propagation, sometimes inducing the formation of rotors. When unstable, they can give rise to ventricular fibrillation, in which synchronous excitation is lost among different parts of the ventricle, impeding contraction, and causing death in a few minutes. To understand this transition, it is necessary to construct models that help us bridge the gap from cellular electrophysiology to propagating properties in tissue, and through whole heart models, to clinical manifestations. This often involves creating very detailed electrophysiological models to study the effect of, for instance, a given mutation. However, the complexity of such models makes sometimes difficult to get insight into the exact arrhythmogenic mechanisms. For this, simplified descriptions can help, as has been the case, for instance, in the study of alternans rhythms. In this talk, we will consider the effects of electro-mechanical coupling in cardiac tissue. We show that mechano-electric models which describe both the electric propagation and the mechanic contraction of the heart naturally lead to close systems of equations with global coupling among the variables. We exemplify this using the Nash-Panfilov model, which reduces to a Fitzgugh-Nagumo type equation with global coupling in the linearly elastic regime. The simplicity of the resulting model allows us to get a better understanding of the different mechano-electric behavior of cardiac tissue both from an analytical and numerical perspective.

A simulation of the life-cycle of myxobacteria

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Myxobacteria swarm forms aggregates that develop into fruiting bodies in response to starvation. We develop an off-lattice model to simulate myxobacteria life cycle, which includes the swarming, the fruiting body and the sporulation stages, based on non-chemotactic cell-cell interactions. We incorporate the Dynamic Energy Budget (DEB) into our model, which successfully links the dynamics of individual cell with the dynamics of the population. In addition, we utilize a logistic equation to model the level of C-signal molecules on each cell surface. Our simulation shows that the coupling of the DEB and the logistic equation can automate the transition from the swarming to the fruiting body stages and also the transitions between the stages of the fruiting body formation, starting from the initial aggregation up to and including the sporulation. Only one parameter, namely the food density, controls the entire life cycle.

Recovering the geometrical properties of a cardiac ischemia: an inverse problem approach

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The objective of this work is to show how we can recover some of the main geometrical properties of a region affected by an ischemia. The cardiac bioelectric activity is simulated in 2-D by a diffusion-reaction equation, where the ischemic region has different electrical behavior than the rest (healthy region). The measurements used to solve the mathematical inverse problem are taken by electrodes placed out of the cardiac membrane.

Competition between Kondo Effect and Reservoir-mediated Superexchange in Double Quantum Dots

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We study a series-coupled double quantum dot in the Kondo regime modeled by the two-impurity Anderson model and find a new conduction-band mediated superexchange interaction that competes with Kondo physics in the strong Coulomb interaction limit. Our numerical renormalization group results, complemented with the higher-order Rayleigh-Schrödinger perturbation theory, show that the novel exchange mechanism leads to clear experimental consequences that can be checked in transport measurements through double quantum dots [1].

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Accelerating numerical solvers using POD+Galerkin projection

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A method will be described to accelerate time-dependent numerical solvers that is based on the combined use of (i) a proper orthogonal decomposition (POD) of some sets of snapshots that are calculated using the numerical solver and (ii) a reduced order model obtained upon Galerkin projection of the governing equations on the POD modes calculated in (i). Now, steps (i) and (ii) are applied in interspersed time intervals. Switching between both is made using an a priori error estimate that provides quite good results. Several improvements will be commented that make the method both robust and computationally efficient. Application will be made to two problems, namely the Ginzburg-Landau equation in transient chaos conditions and the two-dimensional, pulsating cavity problem, which describes the motion of liquid in a box whose upper wall is moving back and forth in a quasi-periodic fashion. In the latter case, the numerical solver will be based on a rough (but quick) computational fluid dynamics (CFD) code that resembles those (industrial) codes that are usually used in Industry. Consequently, it is the numerical code and not the governing equations themselves that is projected into the POD modes. Several consequences of all these will be briefly discussed.

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