Lunes, 17 de enero

Graphene and its unique properties

Prof. Francisco Guinea

CSIC

Abstract

Graphene, two dimensional membrane one atom thick is a novel material which shows features not found previously in other systems. Some of these properties, along with the research erffort which is being carried out in order to elucidate their origin and consequences, will be reviewed.

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Viernes, 28 de enero

Slow pulse due to calcium current induces phase-2 reentry in heterogeneous tissue

Prof. Inmaculada R. Cantalapiedra

UPC

Abstract

Phase-2 reentry is a basic mechanism for the transition to VT and VF in the heart. It is thought to underlie many causes of idiopathic ventricular arrhythmias as, for instance, those occurring in Brugada syndrome. Reentry is usually linked to heterogeneity in tissue repolarization. We study some circumstances under which a region of depolarized tissue can reexcite adjacent regions that exhibit shorter action potential duration (APD), eventually inducing reentry. Simulations are performed using a simplified ionic model that reproduces well the ventricular action potential (AP). We analyze first the conditions that lead to very short action potentials (APs). Then, we show that reexcitation takes place via a slow (calcium current induced) pulse that propagates into the region of short APs until it encounters excitable tissue. In two dimensions, this may give rise to reentry with the formation of counter-rotating spiral waves.

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Miércoles, 2 de marzo

Transmission and Resonance in Photonic Crystal Materials

Prof. Stephanos Venakides

Duke University

Abstract

In the last twenty years, there has been increasing scientific and technological interest in manipulating the propagation properties of light through its interaction with new materials, such as photonic crystals (PC). Typically, these are composite materials, engineered so that their dielectric properties depend periodically on the space variable. They are known also as photonic bandgap materials, a term that derives from gaps that may be present in their continuous EM propagation spectrum.
Our interest lies in the transmission properties of photonic crystal slabs, that display spatial periodicity along the slab and are finite and are possibly repetitive in the incidence direction. We describe resonant behavior and anomalous transmission and we connect this behavior with the existence of guided or leaky EM modes along the PC slab. We derive a generic formula for the description of the asymptotic behavior of the transmission coefficient versus the deviation of the incident frequency from the resonant frequency and the angle of deviation from normal incidence. To understand nonlinear behavior in a rigorous way, we introduce a nonlinear model, retaining critical features, but simplified enough that analytic calculation is possible. We are finally in the process of implementing a 3D boundary integral code for the numerical study of such PC. The code implements the fast calculation of the Green functions in a way that displays superalgebraic convergence. We give most descriptions in the talk, through fields obtained by a 2D code.

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Jueves, 14 de abril

Spin models on random graphs with controlled topologies

Prof. Conrad Pérez Vicente

U. Barcelona

Abstract

We study Ising spin models on finitely connected random graphs drawn from an ensemble which allows for a precise tuning of the topology. We discuss how to solve these models using finite connectivity equilibrium replica theory as well as possible applications of the theory to real-world interacting particle systems.

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Jueves, 5 de mayo

Transiciones de fase en sistemas de osciladores acoplados con espines

Prof. Antonio Prados

U. Sevilla

Abstract

Consideramos un oscilador armónico acoplado linealmente con una cadena lineal de espines. Para un cierto valor de la temperatura, aparece una transición de fase de segundo orden con la posición de equilibrio del oscilador como parámetro de orden. Estudiaremos la dinámica del sistema en dos limites de interés: espines rápidos y oscilador rápido. Asimismo, exploraremos la posibilidad de aplicar este modelo para analizar las curvas fuerza extensión de moléculas biológicas.

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Jueves, 19 de mayo

Meshfree finite dirence methods with minimal positive stencils

Benjamin Seibold

Temple University

Abstract

The finite dirence method is one approach to approximate a partial dirential equation byi a finite dimension problem. An important example is the approximation of the Poisson equation by a large, sparse linear system. While finite dirences are well established for friendly geometries with regular grids, the approach can also be generalized to fully unstructured geometries, and even to disconnected "clouds" of points, which frequently arise in particle methods. Two new aspects come into the game here: first, there are many possible consistent finite diference approximations, and there is no simple principle that defines a "best" one; second, with many classical meshfree approaches, the arising linear systems are in general non-symmetric, do not have an M-matrix structure, and are significantly less sparse than fiite dirence matrices on regular geometries. All of the latter aspects are detrimental for the performance of linear solvers. I will present an approach, based on ℓ^1 optimization, that selects minimal positive stencils, and thus generates optimally sparse M-matrices.

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Jueves, 2 de junio

Effects of stable stratification on wall-bounded turbulent flows

Óscar Flores & Manuel García-Villalba

UC3M

Abstract

Stably-stratified turbulent wall-bounded flows are relevant to many applications in engineering. These flows are characterized by a variation of fluid density in the vertical direction, that often results in strong modifications of the flow patterns by buoyancy. The dynamics of stably-stratified wall turbulence is driven by two competing mechanisms. Vertical motions can extract turbulent kinetic energy from the mean shear but stratification requires them to pay a potential energy toll. Due to the statistical inhomogeneity of wall turbulence, the interplay between these mechanisms can vary significantly with the wall distance in the same flow, specially as the Reynolds number increases. In some cases, the flow even segregates into regions with disparate features, ranging from long velocity streaks in shear-dominated regions to internal gravity waves in buoyancy-dominated regions. In this talk we are going to present results from direct numerical simulations of stably-stratified wall-bounded turbulent flows. Various cases will be presented and discussed, showing the richness and complexity of these flows.

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Viernes, 3 de junio

On the Piloted Ignition of Solid Fuels in Spacecraft Environments

Prof. Sonia Fereres

University of California, Berkeley

Abstract

The effect of environmental variables on the ignition of solid combustible materials is explored through a combination of experimental, analytical and numerical analyses. This research stems from NASA's design requirement to reduce the cabin internal pressure and increase the oxygen concentration in future human space exploration vehicles. These new environmental conditions may result in an increased fire risk of combustible solid materials due to higher flame temperatures (attributed to enhanced oxygen), reduced convective heat losses from heated surfaces and reduced pyrolyzate needed to reach a flammable mixture near the pilot (both attributed to lower pressure). In particular, the influence of low pressure on ignition is emphasized because little is known concerning this topic. A series of experiments conducted in a laboratory-scale combustion wind tunnel with externally irradiated samples of PMMA (polymethylmethacrylate) showed that both the ignition delay time and the fuel mass flux at ignition decrease when the ambient pressure is lowered. An analytical model is used to identify the governing processes that lead to these results and then a numerical model is applied to quantify the influence of ambient variables (particularly pressure) on the piloted ignition of PMMA. The results that will be presented indicate that the flammability of combustible materials is enhanced at low ambient pressures and elevated oxygen concentrations. This may have significant consequences in the assessment of material fire risk in spacecraft and other environments where these conditions are encountered, such as aircrafts and high altitude cities.

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Viernes, 3 de junio

Robust statistical techniques for the analysis of high dimensional gene expression data

Aurora Torrente

UC3M

Abstract

Microarray experiments provide data on the expression level of thousands of genes simultaneously, suggesting several considerable challenges in its pre-processing, management and analysis, that are becoming more and more serious as new high throughput sequencing technologies are being developed. We will describe some robust statistical tools, based on the concept of functional data depth, which measures the centrality of a function within a sample. These techniques include the scale curve, as a way to visualise the dispersion of a set of multivariate observations, and supervised classifications techniques, to assign new observations to one of a given set of (known) groups. These tools are very appropriate for the analysis of high dimensional data, and in particular of microarray data, as its application to real examples has shown. We will also discuss some technical issues that have been taken into account to improve its implementation as a contributed package to the R project, offering the possibilities of using either command-line code or a user-friendly interface.

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Viernes, 17 de junio

Unraveling molecular complexity by manipulating single molecules one at a time

Prof. Felix Ritort

Universidad de Barcelona

Abstract

Recent developments in micro and nano technologies allow for the controlled manipulation of individual molecules by exerting and detecting forces in the piconewton range. The possibility to detect such tiny forces together with the ability of measuring extensions with nanometer resolution allows scientists to monitor molecular reactions in real time (e.g. folding) and characterize thermodynamics and kinetics of individual molecules (e.g. nucleic acids and proteins) within unprecedented accuracy.
In this talk I will review some applications of single molecule experiments to molecular biophysics putting particular emphasis on the use optical tweezers technology to mechanically manipulate single molecules (nucleic acids and proteins). I will also present a few experimental results obtained in our lab on mechanical unzipping of nucleic acids aiming to characterize the energetics of the double helix and the translocation motion of enzymes involved in DNA replication.

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Jueves, 3 de noviembre

Diffusion front capturing schemes for a class of Fokker-Planck equations: Application to the relativistic heat equation

Prof. Antonio Marquina

Universidad de Valencia

Abstract

In this research work we introduce and analyze an explicit conservative finite difference scheme to approximate the solution of initial-boundary value problems for a class of limited diffusion Fokker-Planck equations under homogeneous Neumann boundary conditions. We show stability and positivity preserving property under a Courant-Friedrichs-Lewy parabolic time step restriction. We focus on the relativistic heat equation as a model problem of the mentioned limited diffusion Fokker-Planck equations. We analyze its dynamics and observe the presence of a singular flux and an implicit combination of nonlinear effects that include anisotropic diffusion and hyperbolic transport. We present numerical approximations of the solution of the relativistic heat equation for a set of examples in one and two dimensions including continuous initial data that develops jump discontinuities in finite time. We perform the numerical experiments through a class of explicit high order accurate conservative and stable numerical schemes and a semi-implicit nonlinear Crank-Nicolson type scheme.

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Martes, 8 de noviembre

Coupled phenomena and quantum-continuum coupling in modeling low dimensional nanostructures

Prof. Roderick Melnik

Wilfrid Laurier University

Abstract

Low-dimensional semiconductor nanostructures (LDSNs) are challenging objects to study from both, fundamental physics and mathematical points of view. These objects are receiving increasing attention as key components of many optoelectronic devices. Quantum dots (QDs), LDSNs in which the motion of electrons is confined from all three spatial dimensions, can also be used as biological tags in DNA analysis, as well as in other bio-technological applications, while the idea of using a spin confined to a QD as a qubit promises imminent breakthrough in quantum information processing. The number of practical applications of LDSNs continues to grow which requires the development of adequate mathematical models for their description and efficient numerical approximations.

Despite a wide range of current and potential applications, properties of LDSNs, and QDs in particular, are still frequently analyzed with simplified mathematical models, incapable to account correctly for many effects that are coming from other than quantum mechanical scales (e.g., strain, piezoelectric, thermal and other important effects). In this talk, our main emphasis will be on the mathematical models where the coupling between quantum and continuum mechanics parts is essential. A number of numerical examples will be given to illustrate the theory.

If time permits, we will also discuss new analytical and numerical modelling techniques to control single electron spin states adiabatically through the application of the geometric Berry phase.

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Martes, 15 de noviembre

Graphene as a bridge between high and low energy physics

Prof. M. Ángeles Hernández Vozmediano

Instituto de Ciencia de Materiales de Madrid, C.S.I.C.

Abstract

The main conceptual advances in Physics have usually been prompted by almost simultaneous discoveries in different branches. In the past century, Statistical physics, Quantum Field Theory and Condensed Matter have had their main developments in parallel with the best physicists (Feynman, Landau, Wigner) contributing to them all. Cosmology and astrophysics developed with inputs from Particle Physics. The experimental realization of graphene, a two-dimensional crystal made of carbon atoms in 2004 provides a new and unexpected bridge between Condensed Matter and High-Energy Physics. The low energy excitations of the graphene system are massless Dirac fermions in (2+1) dimensions showing amazing parallelisms with Quantum Electrodynamics. The graphene samples show corrugations that can be modeled with General Relativity techniques. In this talk we will review the main properties of the graphene system using QFT concepts and will show the analogy with General Relativity at work in a few examples. We will also review some on going applications.

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Martes, 22 de noviembre

Homogeneous vapor condensation in boundary layer flows

Mario Durán Camejo

Universidad Carlos III de Madrid

Abstract

Condensation of vapors containing combustion products occurs very often in combustion chambers. These products are typically highly agressive, so subsequent deposition of droplets containing them on chamber walls may result in serious damages. There are other examples where condensation and deposition on a surface is desirable, as in the case of technological processes that produce materials from vaporized substances.

Any case, calculation of deposition rates is very important for regulating its effects, beneficial or not, in many situations in industry.

Condensation of vapor molecules may occur on particles already present inside the chamber or, on the contrary, on clusters produced simultaneously by nucleation of the same molecules. In the first case we talk about heterogeneous condensation and in the last one about homogeneous condensation. Heterogenous condensation in boundary layer flows has been treated extensively on literature, but much less in known in the case of homogeneous condensation.

We propose a thermophysical model for describing homogeneous condensation in laminar boundary layer flows focusing on a stagnation-point flow. The numerical solution of the model provides the spatial profiles of vapor density, droplet density and number of condensate molecules per droplet. In addition we have obtained approximate solutions by using Perturbation Theory techniques which shed new light on the numerical results.

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Jueves, 1 de diciembre

Carbon nanotube-based motor driven by a thermal gradient

Prof. Miguel Rubi

Universidad de Barcelona

Abstract

We present a model able to reproduce experimental observations and computer simulation results of the movement of two coaxial carbon nanotubes induced by a thermal gradient. The model is formulated in terms of a Langevin equation which includes the friction force, the van der Waals forces between both nanotubes, that depend on their chiralities, and the inhomogeneous temperature distribution which give rise to an inhomogeneous phonon distribution. The random force term is assumed to be related to the fluctuations of the heat current along the inner nanotube and therefore its intensity is proportional to the heat conductivity. The model reproduces the rich variety of possible dynamic behaviors and proves the conjecture that the driving force is the phononic current induced by the thermal gradient. Applications to other nano-electromechanical devices are also analyzed.

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Lunes, 5 de diciembre

Higher-order averaging of linear Fokker-Planck equations

Stephan Martin

Universidad de Kaiserslautern

Abstract

Energy dynamics of stochastic Hamiltonian systems can be investigated by the method of stochastic averaging. If the mechanical system is under additional periodic forcing, say friction, the energy dynamics and equilibria will change. These small deviations in energy cannot be captured by classical stochastic averaging. We present a method of higher-order averaging based on an asymptotic expansion of equilibria, which is able to (numerically) generate averages in the subtle limit of small noise and small friction. The influence of periodic forcing will become visible only to second order. We present our method and its results for standard oscillators as well as an application to fiber dynamics.