Jornadas de Investigación del Instituto Gregorio Millán Barbany

Universidad Carlos III de Madrid
Días 19 y 20 de enero de 2017

19 de enero: Mecánica de Fluidos e Ingeniería Aeroespacial

10:00	A. Liñán
10:45	Café
11:20	P. L. Garcia-Ybarra
12:00	J. Rodriguez Rodriguez
12:40	S. Le Clainche
13:20	O. Flores
14:00	Comida
15:15	J.L. Castillo
15:55	P. A. García-Salaberri
16:35	Café
16:55	M. Sanjurjo Rivo
17:35	M. Lara

20 de enero: Materia Condensada/Nano

9:30	G. Platero
10:10	L. Viani
10:50	Café
11:10	J. Christensen
11:50	A. Lasanta
12:30	C. Kanyinda-Malu
13:10	M. Ruiz-Garcia
13:30	Comida
15:00	A. Prados
15:40	F. Vega Reyes
16:20	R. Sánchez
17:00	Clausura

Structure of granular materials formed by depositing nanoparticles generated from electrosprayed liquid suspensions

J.L. Castillo, S. Martin, D. Rodriguez-Perez and P.L. Garcia-Ybarra

Departamento de Fisica Matemática y de Fluidos, Facultad de Ciencias, Universidad Nacional de Educacion a Distancia (UNED). Madrid 28040, Spain

The preparation of nanostructured materials from the deposition of electrosprayed liquid suspensions leads to granular deposits whose roughness and porosity should be properly controlled as these morphological deposit features play a crucial role in many practical applications. This is the case of the performance of such materials when used as catalytic enhancers (Martin *et al*, 2010, Martin *et al*, 2013, Castillo *et al*, 2014). Subtle changes in the liquid composition and in the electrospray working parameters affect the stability of the cone-jet mode (Martin *et al*, 2012) and therefore influence the particle arrival to the collecting surface which indeed determine the deposit structure (Rodriguez-Perez *et al*, 2005, 2007).

An experimental work has been performed aiming to characterize and to control the structure of fuel cell electrodes formed by Pt/C nanoparticles and ionomer (Nafion®). For these applications, a proper combination of nanoparticles and Nafion in the electrodes is needed to accommodate the electronic and protonic currents in the fuel cell whereas a large porosity is required to achieve a large exposition of catalytic active sites to the reacting gases. A suspension of nanoparticles and Nafion in ethanol is electrosprayed toward a collecting surface where the solid residue forms a porous structure. All the particles emitted at the electrospray tip are collected on the substrate. Therefore, the relative amounts of the solid constituents are the same in the liquid suspension as in the deposit. Changes in the relative amount of Nafion (% of weight of Nafion with respect to the total amount of carbon, platinum and Nafion in the liquid suspension) modify the liquid conductance and promote noticeable differences on the deposit structure.

The dependence of the deposit mean porosity on the Nafion content has been analyzed. The enclosed figure gathers some SEM images of deposits formed with $20\%_{wt}$ Nafion (images a&c) and $50\%_{wt}$ Nafion (b&d) and the same total mass. It becomes clear that the building blocks of the material formed with the higher amount of Nafion (SEM images b&d in the figure) are smaller aggregates which consist of a lower number of nanoparticles (see top views a&b). Moreover, for $50\%_{wt}$ Nafion the deposit is much higher (see cross section views, c&d), and, as a consequence, its porosity is even larger.

As a conclusion, the electrodynamic atomization of liquid suspensions can be used to control the porosity of nanostructured materials according to the application needs.

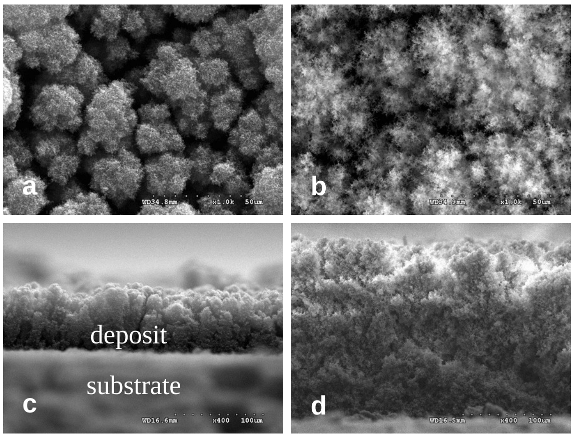

Figure. Top view (a&b) and cross section (c&d) SEM images of granular deposits from suspensions containing 20%wt Nafion (a&c) and 50%wt Nafion (b&d) with the same total mass (5.7 mg) deposited on a 5 cm^2 colleting surface.

Work supported by Ministerio de Economía y Competitividad (Spain) under project ENE2015-67635-R.

References:

Castillo, J.L., Martin, S., Rodriguez-Perez, D., Perea, A., Garcia-Ybarra, P.L. (2014) *KONA Powder and Particle Journal*. **31**, 214-233.
Martin, S., Garcia-Ybarra, P.L., Castillo, J.L. (2010) *J. Power Sources.* **195**, 2443-2449.
Martin, S., Garcia-Ybarra, P.L., Castillo, J.L. (2010) *Int.J. Hydrogen Energy.***35**, 10446-10451.
Martin, S., Martinez-Vazquez, B., Garcia-Ybarra, P.L., Castillo, J.L. (2013) *J. Power Sources.* **229**, 179-184.
Martin, S., Perea, A., Garcia-Ybarra, P.L., Castillo, J.L. (2012) *J. Aerosol Sci*. **46**, 53-63.
Rodriguez-Perez, D., Castillo, J.L., Antoranz, J.C. (2005) *Phys. Rev. E*, **72**, 021403.
Rodriguez-Perez, D., Castillo, J.L., Antoranz, J.C. (2007) *Phys. Rev. E*, **76**, 011407.

Phononic Metamaterials

Johan Christensen
G. Millán Institute, Fluid Dynamics, Nanoscience and Industrial Mathematics, Universidad Carlos III de Madrid, Leganés, Spain

The boost experienced by acoustic and mechanical (phononic) metamaterial research during the past years has been driven by the ability to sculpture the flow of sound waves at will. Motivated by the desire to engineer artificial structures in the form of metamaterials and the quest to map quantum mechanical phenomena onto classical waves such as sound has led to vast possibilities in material designs for control of wave motion and the potential for engineering applications. Some striking material properties have shown in the past to be able to leave an objective acoustically concealed, hence they are cloaks of “unhearability”. Also, fascinating materials have been designed to be able to bend a ray of sound the “wrong” way when, for example, a loudspeaker turned on irradiates such artificial structure with a negative refraction index. In this talk, I like to review some of the key achievements made in this field and wish to address some of the unanswered questions that might lead to a breakthrough in the future.

Three-dimensional instabilities in the wake of an infinite aspect ratio flapping wing at low Reynolds number

O.Flores & M. Garcia-Villalba
Dept. Bioingenieria e Ing. Aeroespacial, UC3M.

The aerodynamics of flapping wings has received a lot of attention in the last years, driven by the interest in the development of bio-inspired Micro Air Vehicles with flapping wings, with sizes comparable to small birds or insects. Although there are several successful designs of these flappers, there are still a number of issues precluding their systematic design. One of these issues is the better understanding of the unsteady aerodynamics associated to the leading edge vortex. The work that I am going to present in this seminar investigates the importance of 3D effects, analyzing the effect that the stability of the wake has on the performance of a plunging and pitching wing of infinite aspect ratio. Four kinematics with large amplitudes and low Reynolds are analyzed using two and three-dimensional Direct Numerical Simulation (DNS), as well as a Floquet stability analysis of the 2D cases. This analysis will show that only one case shows an absolute instability, while the others exhibit a convective instability that is unable to maintain a three dimensional wake downstream of the airfoil. Besides that, the comparison of the 2D and 3D simulations shows that the presence of a 3D wake at this Reynolds number has a small impact on the aerodynamic forces.

Limitations of Volume-Averaged Formulation of Gas Diffusion Layers in the Modeling of Polymer Electrolyte Fuel Cells

Pablo A. García-Salaberri*, Marcos Vera*, Jeff T. Gostick†, Gisuk Hwang‡,

Iryna Zenyuk• and Adam Z. Weber○

* Dpto. de Ingeniería Térmica y de Fluidos, Universidad Carlos III de Madrid, Leganés, Spain
e-mail: pagsalab@ing.uc3m.es, mvcoello@ing.uc3m.es - web page:
http://fluidosuc3m.es/research/microfluidics/

† Department of Chemical Engineering, McGill University, Montreal, Quebec, Canada
e-mail: jeff.gostick@mcgill.ca - web page: http://pmeal.com/

‡ Department of Mechanical Engineering, Wichita State University, Wichita, Kansas, USA
e-mail: Gisuk.Hwang@wichita.edu - web page: http://webs.wichita.edu/?u=gshwang

• Department of Mechanical Engineering, Tufts University, Medford, Massachusetts, USA
e-mail: iryna.zenyuk@tufts.edu - web page: http://engineering.tufts.edu/me/people/Zenyuk/

○ Energy Conversion Group, Lawrence Berkeley National Laboratory, Berkeley, California, USA
e-mail: azweber@lbl.gov - web page: https://eetd.lbl.gov/people/adam-weber

ABSTRACT

Numerical modeling plays a crucial role for the analysis of the complex multiphysics, multiphase and multiscale transport phenomena that take place in the membrane electrode assembly of Polymer Electrolyte Fuel Cells (PEFCs). In particular, thorough understanding of the coupled mass, charge and heat transport processes that occur in thin, heterogeneous, anisotropic, mix-wettability Gas Diffusion Layers (GDLs) is essential to develop novel fuel-cell designs with improved performance and extended durability. In this work, various techniques, such as continuum, lattice Boltzmann and pore network methods, are combined with X-ray tomographic reconstructions of dry and partially-saturated GDLs to perform numerical simulations on the material microstructure [1, 2]. The effects of GDL pore-scale architectures on cell performance and effective transport properties (diffusivity, permeability, and electrical and thermal conductivity) are examined. In addition, the limitations introduced by the widely used volume-averaged approach when modeling finite-size GDL materials are discussed. For this purpose, the predictions of a 3D PEFC model using a fully volume-averaged description are compared with those accounting for the real GDL microstructure. The insight gained from this work-in-progress will be leveraged to develop advanced PEFC models in order to assist the construction of next-generation GDLs, as well as to improve our understanding of PEFC technology.

REFERENCES

[1] P. A. García-Salaberri, G. Hwang, M. Vera, A. Z. Weber, J. T. Gostick, "Effective diffusivity in partially-saturated carbon-fiber gas diffusion layers: Effect of through-plane saturation distribution", *Int. J. Heat Mass Tran.*, Vol. **86**, pp. 319–333, (2015).

[2] P. A. García-Salaberri, J. T. Gostick, G. Hwang, A. Z. Weber, M. Vera, "Effect of local saturation and application to macroscopic continuum models", *J. Power Sources*, Vol. **296**, pp. 440–453, (2015).

Experimental characterization of laminar jet flames of methane-air mixtures subjected to strong curvatures

Gabriel Garcia-Soriano[1], Sergio Margenat[1], Francisco J. Higuera[2], Jose L. Castillo[1] and Pedro L. Garcia-Ybarra[1]

[1] *Dept. Fisica Matematica y de Fluidos, UNED, Senda del Rey 9, 28040 Madrid, Spain*

[2] *ETSIAE, Universidad Politeccnica de Madrid, Plaza Cardenal Cisneros 3, 28040 Madrid, Spain*

Abstract

An experimental setup has been developed to investigate the correlation between local burning velocity and flame stretch in laminar jet flames of methane-air mixtures at different equivalence ratios. Gas flow velocities were obtained by PIV (Particle Image Velocimetry) from images of axial sections of seeded flames and the location of the flame front was related to the gradient of luminosity. Flame stretch was determined and shown to be mainly due to flame curvature whereas the gas velocity strain has a small contribution. *Low* inlet gas velocities lead to short rounded flames and the classical Markstein relation was experimentally validated at any point of the flame fronts. However, for *large* blowing velocities that can be one order of magnitude larger than the planar flame velocity, the flames adopted slender quasi-conical shapes. Far from the flame tip, these flames are quasi-planar and obey the Markstein linear relation whereas, when the tip region is approached by distances on the order of the Markstein length, a strongly nonlinear behavior is observed. Furthermore, in this non-linear region, the local values of the flame stretch turn out to be no longer enough to determine the burning velocities univocally and the value of the inlet gas velocity has also to be prescribed. These results have been analyzed by adding a quadratic term to the Markstein linear relation. The coefficient affecting this new term depends on the blowing intensity and appears to be well fitted by a square root law of the difference between the actual value of the blowing velocity and some critical value below which this term vanishes and the Markstein relation holds. This kind of sharp transition is reminiscent of a classical critical behavior and could be tentatively ascribed to a threshold of stability exchange between rounded (weakly curved) flames and slender (strongly curved) flames that is controlled by the inlet gas velocity.

OPTICAL PROPERTIES OF NEGATIVE INDEX MATERIALS: USE OF SEMICONDUCTOR NANOSHELLS AS LOSS FREE OR ACTIVE PLASMONIC NIM'S.

Authors: CLEMENT KANYINDA-MALU KABIENA, Rosa M. DE LA CRUZ and JUAN E. MUÑOZ-SANTIUSTE

Abstract:

Since the prediction that a material with negative index of refraction can be used to construct perfect lens, a quest for media that possesses a negative index has been probed in a wide range of metamaterials. Negative index materials, also known as left-handed materials, has negative permittivity and permeability simultaneously.

Most of commonly used or employed systems to assess on negative index metamaterials have been focused in designing or simulating devices with periodically repeated multilayers. Indeed, such designs present one-dimensional waveguides where properties that lead the refractive index may change from positive to negative values, depending on the layered structures. Most of these metamaterials are made up of metallic nanoparticles, either in layers or completely embedded in the matrix of semiconductors. Many attempts to design NIMs materials in 3-dimensional geometry is still under research.

Actually, many other materials such $LiNbO_3$ are also used to create negative index materials, out of the all known metallic-semiconductor multilayers. During this talk, we will try to review the basic key properties of negative index metamaterials and why these materials have received extensive attention. We will also try to explain how we come to the use of semiconductor nanoshells systems to account of negative permittivity using simple dielectric continuum models.

Exploring sensitivity of orbital dynamics with respect to model truncation. The frozen orbits approach.

Martin Lara
GRUCACI – University of La Rioja
Space Dynamics Group – UPM

Abstract: In orbit determination problems the mathematical model used must be as close to the actual dynamics as possible. On the contrary, accuracy constraints can be notably relaxed for orbit prediction purposes. We focus on perturbed Keplerian motion and explore how to ascertain the correct truncation of the dynamical model by investigating relevant particular solutions of the problem: the so-called frozenorbits.

Efecto Mpema en medios granulares: ¿se puede enfriar más rápidamente lo que está más caliente?

A. Lasanta[1,2], F. Vega Reyes[1,3], A. Prados[4], A. Santos[1,3]

[1]Departamento de Física, Universidad de Extremadura, 06071 Badajoz, Spain

[2]G. Millán Institute, Fluid Dynamics, Nanoscience and Industrial Mathematics, Universidad Carlos III de Madrid, 28911 Leganés, Spain and Department of Materials Science and Engineering and Chemical Engineering, Universidad Carlos III de Madrid, Leganés, Spain

[3]Instituto de Computación Científica Avanzada (ICCAEx), Universidad de Extremadura, 06071 Badajoz, Spain

[4]Física Teórica, Universidad de Sevilla, Apartado de Correos 1065, E-41080 Sevilla, Spain

El **efecto Mpemba** se produce cuando tenemos dos recipientes de agua uno a temperatura Tc, otro a Tf, con Tc>Tf, y el más caliente se enfría antes [1]. Ésto es bien conocido en aquellos países donde se alcanzan temperaturas muy bajas en invierno. A lo largo de la historia aparecen afirmaciones que hacen referencia a esta paradoja, de Aristóteles, Francis Bacon, Roger Bacon y Descartes entre otros, por ejemplo:

> "*Si el agua ha sido previamente calentada, esto contribuye a la velocidad a la que se enfría: lo hará más rápidamente…*" Aristóteles 350 A. C.
> "*…, si agua caliente y agua fría se colocan en dos recipientes, el agua se congelará más rápidamente…*" Roger Bacon siglo XIII.

Este efecto tan particular empezó a ser estudiado rigurosamente a partir de los experimentos llevados a cabo por Erasto B. Mpempa [2] en la década de los 60, y con cuyo nombre se conoce popularmente. El efecto "clásico" se produce al enfriar un líquido en contacto con un reservorio térmico. Se le han atribuido diferentes y complejas explicaciones, tales como la evaporación, flujos internos, gradientes y la influencia del superenfriamiento, así como combinaciones de éstas. Además, ha sido observado en diversos materiales, como por ejemplo en nanotubos de carbono y aleaciones.

En esta charla mostraremos que el efecto Mpemba está presente en fluidos granulares, tanto en el caso de enfriamiento homogéneo como en el caso uniformemente calentado. En ambos casos el sistema permanece homogéneo e isótropo, no aparecen transiciones de fase y tiene la particularidad de estar fuera del equilibrio. A su vez, presentaremos predicciones analíticas cuantitativas de cómo deben de ser preparados los estados iniciales a diferentes temperaturas para que el efecto Mpemba tenga lugar y serán comparadas con resultados numéricos de simulación [3] . Esto nos proporcionará una explicación clara al efecto en éste tipo de sistemas y abrirá la puerta a posibles implicaciones de nuestro análisis a otros casos.

[1] M. Jeng, Am. J. Phys. 74, 514 (2006).
[2] E. B. Mpemba and D. G. Osborne, Phys. Educ. 4, 172 (1969).
[3] A. Lasanta, F. Vega Reyes, A. Prados, A. Santos arXiv preprint arXiv:1611.04948 (under review)

HIGHER ORDER DYNAMIC MODE DECOMPOSITION

S. Le Clainche & J.M. Vega

Department of Applied Mathematics, School of Aerospace Engineering,

Universidad Politécnica de Madrid

Dynamic Mode Decomposition (DMD) [1] is a well-known technique suitable to study flow dynamics and structures, that is based on seminal results of the Koopman operator theory [2]. This technique describes the flow dynamics as a linear combination of exponential terms, so successfully results are obtained when the analysis is performed in either linear laminar flows or in complex flows with similar spectral and spatial complexity. However, DMD is sensitive to the collected data and the transient flow trajectory. Thus, the method does not always give the expected results when the data collected are noisy and complex, or when the spatial complexity is smaller than the spectral complexity. We present a new more general DMD-like algorithm, called Higher Order Dynamic Mode Decomposition (HODMD) [3], in order to address such problems. The performance of this method has been tested in several cases in which DMD performance is not optimal or even fails, including results obtained from Ginzburg-Landau or Navier-Stokes equations, in highly noisy PIV experimental data describing transitional flow and to study the thermal convection in a rotating spherical fluid shell subject to radial gravity. This algorithm will also be compared with classical methods commonly used in experimental analysis such as Fast Fourier Transform (FFT) or Power Spectral Density (PSD), showing its outperformance.

References

[1] P. J. Schmid, Dynamic mode decomposition of numerical and experimental data, J. of Fluid Mech. 656(2010), 5–28.

[2] B. Koopman, Hamiltonian systems and transformations in Hilbert space, Proc. Natl Acad. Sci. USA 17(1931), 315–318.

[3] S. Le Clainche, J.M. Vega, Higher order dynamic mode decomposition, SIAM J. of Appl. Dyn. Sys., (*In press*).

Contribución de Gregorio Millán Barbany al papel de la Mecánica de Fluidos en el desarrollo de la Aeronáutica

Amable Liñán
ETSIAE, Universidad Politeccnica de Madrid,
Plaza Cardenal Cisneros 3, 28040 Madrid, Spain

Long range transfer in quantum dot arrays

Gloria Platero
Instituto de Ciencia de Materiales de Madrid - CSIC

Recent experiments in semiconductor triple quantum dots show clear evidence of charge and spin electron exchange between the outermost dots. I will discuss long-range transport and quantum interferences in ac driven triple dots where transitions between distant and detuned dots are mediated by the exchange of photons. We propose the phase difference between the two ac voltages as an external parameter, which can be easily tuned to manipulate the current characteristics.
I will also discuss the effect of topology and driving in the electron dynamics in arrays of quantum dots forming a chain of dimers.

Non-conservative interacting systems: on the global stability of their non-equilibrium steady states

A. Prados*

Física Teórica, Universidad de Sevilla, Apdo. de Correos 1065, Sevilla 41080, Spain

(Dated: January 10, 2017)

In kinetic theory, a system is described by its one-particle distribution function $f(\boldsymbol{r}, \boldsymbol{v}, t)$, such that $f(\boldsymbol{r}, \boldsymbol{v}, t) d\boldsymbol{r} d\boldsymbol{v}$ is the fraction of particles with positions and velocities in the intervals $(\boldsymbol{r}, \boldsymbol{r} + d\boldsymbol{r})$ and $(\boldsymbol{v}, \boldsymbol{v} + d\boldsymbol{v})$, respectively. In systems with non-conservative interactions, such as granular fluids, the global stability of the non-equilibrium steady states and the possible existence of an associated Lyapunov functional (that is, an H-theorem) are open problems.

Here, we address the above issue in the framework of a lattice model for granular-like velocity fields. For a quite general driving mechanism, including both boundary and bulk driving, we show that the steady state reached by the system in the long time limit is globally stable. This is done by proving analytically that a certain H-functional is non-increasing in the long time limit. Moreover, for two specific, physically relevant, energy injection mechanisms, we are able to demonstrate that the proposed H-functional is non-increasing for all times.

Furthermore, we also illustrate the reason why the "classical" Boltzmann functional $H_B[f] = \int d\boldsymbol{r}\, d\boldsymbol{v} f(\boldsymbol{r}, \boldsymbol{v}, t) \ln f(\boldsymbol{r}, \boldsymbol{v}, t)$ is inadequate for systems with non-conservative interactions. Not only is this done for simple lattice models but also for systems having a quite general kinetic description, like the Boltzmann or Enskog equation.

* prados@us.es

Dip coating of a flat plate immersed in a fluid bath containing two immiscible fluids

Javier Rodríguez Rodríguez, UC3M
Alexander Korobkin, University of East Anglia (UK) y catedrático de excelencia UC3M
Benoit Scheid, Universidad Libre de Bruselas (BE)

A vertical plate lifted from a bath of a viscous fluid drags with it a thin film of liquid when the exit speed exceeds a critical value. This is the well-known Landau-Levich-Derjagin flow, which is of relevance in coating applications.

We have revisited this problem for the case when there exists a layer of a immiscible fluid on top of the bath (such as oil on water). Different configurations may appear depending on the interplay between the two contact lines (liquid-liquid-gas and liquid-solid-gas). Perhaps the most interesting one, form the point of view of coating applications, is that when the lower liquid perfectly wets the plate whereas the upper one does not. We will show how this configuration allows to control the thickness of the deposited layer in a flexible and practical way.

Characterizing and Enhancing Chaotic Behavior in Semiconductor Superlattices

Miguel Ruiz-Garcia, Luis L. Bonilla, Manuel Carretero

G. Millán Institute, Fluid Dynamics, Nanoscience and Industrial Mathematics and Department of Materials Science and Engineering and Chemical Engineering, Universidad Carlos III de Madrid, Leganés, Spain

Fast spontaneous chaotic oscillations are used to generate high-quality true random sequences in random number generators. Using fast practical sources of entropy to produce true random sequences is crucial to make storage and transfer of data more secure at very high speeds [1]. Secure communications and e-commerce come to mind. While the first high-speed physical sources of entropy were chaotic semiconductor lasers [2], the discovery of spontaneous chaos in semiconductor superlattices (SSL) at room temperature provides a valuable all-electronic nanotechnology alternative [3].
Analysis and numerical simulations of appropriate superlattice models are needed to understand spontaneous chaos at room temperature. So far, only idealized models of superlattices having identical periods have been studied. Spontaneous chaos in the current through the superlattice occurs when it is biased in narrow dc voltage ranges near sharp transitions between different current oscillation modes [4]. When the superlattice is biased in a voltage region close to the transition between stationary and time periodic current, we have shown that external noise added to dc voltage bias may produce non-periodic chaotic current signals [5]. In addition, we will discuss the mechanism that originates deterministic chaotic behavior in SSLs, and different superlattices configurations that may enhance the chaotic behavior [6].

[1] T.E. Murphy and R. Roy, The world's fastest dice, Nature Photonics 2, pp. 714-715 (2008).

[2] A. Uchida, K. Amano, M. Inoue, K. Hirano, S. Naito, H. Someya, I. Oowada, T. Kurashige, M. Shiki, S. Yoshimori, K. Yoshimura and P. Davis, Fast physical random bit generation with chaotic semiconductor lasers, Nature Photonics 2, pp. 728-732 (2008).

[3] W. Li, I. Reidler, Y. Aviad, Y. Huang, H. Song, Y. Zhang, M. Rosenbluh and I. Kanter, Fast Physical Random-Number Generation Based on Room-Temperature Chaotic Oscillations in Weakly Coupled Superlattices, Phys. Rev. Lett. 111, 044102 (2013).

[4] M. Alvaro, M. Carretero and L.L. Bonilla, Noise enhanced spontaneous chaos in semiconductor superlattices at room temperature, Europhys. Lett. - EPL 107, 37002 (2014).

[5] Z. Yin, H. Song, Y. Zhang, M. Ruiz-García, M. Carretero, L. L. Bonilla, K. Biermann and H. T. Grahn, Noise-enhanced chaos in a weakly coupled GaAs/(Al,Ga)As superlattice, Phys. Rev. E, (in press)

[6] M. Ruiz-Garcia, J. Essen, M. Carretero, L. L. Bonilla, and B. Birnir, Enhancing chaotic behavior at room temperature in GaAs/(Al,Ga)As superlattices, submitted to Physical Review B.

Chiral heat currents in the quantum Hall regime

Rafael Sánchez
Universidad Carlos III de Madrid

In an electronic circuit, current can be generated by the conversion of heat absorbed from a hot region. In the absence of a magnetic field, such thermoelectric response requires broken left-right and particle-hole symmetries. We investigate the thermoelectric properties of a three-terminal quantum Hall conductor. We show that thermoelectric measurements are sensitive to the chiral nature of the quantum Hall edge states, opening the way to control quantum coherent heat flows. Chiral dependent effects include extreme asymmetries of the Onsager coefficients, a thermoelectric response in spatially symmetric configurations, or the possibility to generate spin-polarized currents in quantum spin Hall samples [1]. Also, powerful and efficient energy harvesters can be proposed [1,2].

The effect of the chiral propagation affects the heat currents as well. This results in huge thermal rectification coefficients in three terminal configurations, which operate as ideal heat diodes [3].

References:
[1] R. Sánchez, B. Sothmann, A. N. Jordan. Phys. Rev. Lett. 114, 146801 (2015)
[2] B. Sothmann, R. Sánchez, A. N. Jordan, Europhys. Lett. 107, 47003 (2014)
[3] R. Sánchez, B. Sothmann, A. N. Jordan. New J. Phys. 17, 075006 (2015)

Periodic solutions in the optimal control problem of wind power generation with kites

Manuel Sanjurjo Rivo
Bioengineering and Aerospace Engineering Dpt., Instituto Gregorio Millán.

The utilisation of kites at high altitude allows us to extract energy from winds at high speed. Many possible configurations and system solutions have been proposed in the past years, but all of them involve the operation in a pumping orbit. Part of the pumping cycle requires an energy input, whereas the power generation occurs in the rest of the orbit. It is therefore mandatory to optimise the pumping cycle in order to get an economically profitable operation of the kite. An optimal control problem (OCP) can be set up given a particular dynamical model of the kite. Here, a simple dynamical model of the kite is considered as well as a single and simple control.

The indirect approach to the OCP recasts it as a boundary value problem. When the solution is known to be periodic, the problem is equivalent to searching for periodic solutions in a dynamical system that doubles the dimension of the original, physical one. In this work, we explore the possibility to exploit this fact in order to compute efficiently optimal pumping cycles in terms of energy production.

Inherent thermal convection for a fluid inside a box

Francisco Vega Reyes, Andrea Puglisi, Giorgio Pontuale and Andrea
Gnoli

In this work we show the conditions for the existence of an inherent mechanism of thermal convection. That is, convection does not have a critical value because it is always present, constituting the base steady state (the simplest steady state) of a fluid delimited inside a rectangular region by four walls. Two of the parallel walls act as sinks of thermal energy and the other two as sources of thermal energy. When there is also a gravitational field, and regardless of whether the heating of the fluid is done from "up" or "down" (the classical Bénard convection only appears when the heating is from below). The study is done via four independent methods: hydrodynamic theory, Monte Carlo simulations of the kinetic equation of a gas, simulations of molecular dynamics and experiments of a granular system (macroscopic particles). We show the validity of the Boussinesq equations for the case of small gravity.

Resonant Energy Transport in Dye-Filled Monolithic Crystals of Zeolite L: Modeling of Inhomogeneity

Lucas Viani
G. Millán Institute, Fluid Dynamics, Nanoscience and Industrial Mathematics, Universidad Carlos III de Madrid, Leganés, Spain

Resonant energy transfer (RET) is a key mechanism in organic optoelectronic devices, and its efficiency depends critically on the intermolecular arrangement of the active com-pounds. Supramolecular organization promoted by nanostructured supramolecular host-guest compounds (HGCs) is an elegant way of controlling the packing of the molecules inserted in optically inert organic or inorganic host materials. Under ideal conditions (i.e. dye properties and homogeneous distribution) very high exciton diffusion rates are expected in Zeolite L HGCs, being of high relevance for practical applications. From experiment however, there is clear evidence for inhomogeneity dependent on the type of the chromophores, the preparation procedure, and the size of host crystals, but the reason for inhomogeneity and the consequences on exciton diffusion are under debate. In this work we elucidate these issues making use of computational tools (dynamic Monte Carlo and molecular dynamics) to elucidate the RET dynamics in the inorganic Zeolite L taking into account the inhomogeneity of the dye distribution along the 1D channels.