Maths & chemistry

Zaragoza (Spain), June 20-22, 2012

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Pedro J. Miana
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Instituto Universitario de Investigación de Matemáticas y Aplicaciones Universidad Zaragoza
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GOBIERNO DE ARAGON
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Workshop Maths & Chemistry
Zaragoza, June 20-22, 2012

Queridos compañeros:

Cerramos con este Workshop Maths & Chemistry 2012, la serie de congresos científicos que el Instituto Universitario de Matemáticas y Aplicaciones, IUMA, comenzó con Maths & Water 2008 y que anualmente se ha dedicado a los elementos Fuego (2009), Aire (2010) y Tierra (2011).

Mantenemos el esquema de tres días de trabajo con conferencias invitadas e impartidas por reconocidos investigadores nacionales e internacionales. También se han aceptado las solicitudes de presentaciones cortas y de pósteres.

Los temas que se tratarán son diversos, desde la modelización matemática de fenómenos químicos, hasta la simulación numérica de reacciones químicas; las conexiones entre matemáticas y nanotecnología; combustiones y dinámica; o las ecuaciones para la formación de líquidos poliméricos.

Agradecemos el excelente trabajo realizado por el Comité Científico y las facilidades prestadas por la Facultad de Ciencias, la Universidad de Zaragoza y el Gobierno de Aragón para la realización de este congreso.

Confiamos en contar con su presencia para que esta reunión científica sea un éxito.

Equipo directivo del IUMA

Juan Ignancio Montijano
Luis Rández
Pedro J. Miana

Maths & Chemistry, June 2012, 20-22

	Wednesday 20 June	**Thursday 21 June**	**Friday 22 June**
09.30-09.50	*Registration*	Turgay Uzer	Manuel G. Velarde
10.00-10.25	*Opening Ceremony*		
10.30- 11.25	Herschel A. Räbitz	Jesús Palacián	Alejandro Toro-Labblé
11.30-11.55	*Coffee-Break*	*Coffee-Break*	*Coffee-Break*
12.00-12.55	Jesús Ildefonso Díaz	Tim Myers	Guillermo Hauke
13.00-13.55	Bernardo Herradón	Miguel A. Herrero	*Closing Ceremony*
	Lunch	*Lunch*	*Lunch*
16.30-16.55	Chelo Ferreira		
17.00-17:25	Luca Bergamasco		
17.30-17.55	Laura Usón		
18.00-18.25	*Coffee-Break*		
18.30-18.55	Alberto Vergel	*19 h.Guide visit Zaragoza (2 hours)*	
19.00-19.30	Ignacio Julián		

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Time Schedule

Wednesday, June 20th

Sala de Grados, Faculty of Sciences

09.30–09.50 Registration

10.00–10.25 Opening Ceremony

10.30–11.25 H. Räbitz, University of Princeton
Control of Phenomena in the Sciences over Vast Length and Time Scales

11.30–11.55 *Coffee break*

Room 12, Faculty of Sciences

12.00–12.55 J. Ildefonso Díaz, Universidad Complutense de Madrid
On the Ostwald ripening phenomenon in reactive batch crystallizers and other chemical reaction processes

13.00–13.55 B. Herrandón, CSIC
Maths and chemistry, a necessary relationship: A historical perspective and some current results from computational chemistry

14.00–16.25 *Lunch Break*

Room 12, Faculty of Sciences

16.30–16.55 C. Ferreira, Universidad de Zaragoza
Two different mathematical contributions to chemistry: Special functions and Regression Models.

17.00–17.25 L. Bergamasco, ITA,
Lattice Boltzmann solution of FENE constitutive equations for polymeric liquids

17.30–17.55 L. Usón, INA,
Numerical simulation of the synthesis of iron nanoparticles prepared in a laser pyrolysis reactor

18.00–18.25 *Coffee break*

18.30–18.55 A. Vergel, Universidad Politécnica de Madrid
Isomerization system LiCN/LiNC: Geometrodynamical version

19.00–19.25 I. Julián, Universidad de Zaragoza
A modified Counter Current Back Mixing (CCBM) model to predict the solid axial mixing in a Two Section & Two Zone Fluidized Bed Reactor

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Thursday, June 21 th

Room 12, Faculty of Sciences

09.30–10.25 T. User, Georgia Institute of Technology
Transition state theory: The phase space perspective

10.30–11.25 J. Palacián, Universidad Pública de Navarra
Mathematical foundations of the transition state theory

11.30–11.55 *Coffee break*

12.00–12.55 T. Myers, CRM
Mathematics and Nanotechnology

13.00–13.55 M.A. Herrero, Universidad Complutense de Madrid
A few mathematical problems inspired by Chemistry

14.00–16.30 *Lunch Break*

19.00–21.00 *Short visit to Zaragoza*

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Friday, June 22 th

Room 12, Faculty of Sciences

09.30–10.25 Manuel G. Velarde, Universidad Complutense de Madrid
Model studies of electron transfer and conduction mediated by solitons in 1D and 2D crystal lattices

10.30–11.25 A. Toro-Labblé, Pontificia Universidad Católica de Chile
Mathematical Characterization of Chemical Reactions and Molecular Properties

11.30–11.55 *Coffee break*

12.00–12.55 G. Hauke, Universidad de Zaragoza
Combustion processes and cavitating bubble dynamics

13.00–16.30 *Lunch Break*

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Control of Phenomena in the Sciences over Vast Length and Time Scales

Professor Herschel Rabitz
Department of Chemistry
Princeton University

The control of physical, chemical, and biological phenomena are pervasive in the sciences. The dynamics involved span vast length and time scales with the associated controls ranging from shaped laser pulses out to the application of special chemical reagents and processing conditions. Despite all of these differences, there is clear common behavior found upon seeking optimal control in these various domains. Evidence of this common behavior will be presented from the control of quantum, chemical, and biological processes. The most evident finding is that control efforts can easily beat the so-called curse of dimensionality upon satisfaction of assumptions that are expected to widely hold. The potential consequences of the observations will be discussed.

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On the Ostwald ripening phenomenon in reactive batch crystallizers and other chemical reaction processes

J.I. Diaz

The lecture will be divided in two different parts: the first part (of a more expository nature) will be devoted to the illustration of some time periodic chemical processes (the Beloussov- Zhabotinski reaction). In contract to that, in a second part (containing original researchers by the author) we shall show how very often some of the chemical reactions takes place in a very short time and only one of them remains active for long time: it is the so called Ostwald ripening phenomenon.

Keywords: Beloussov- Zhabotinski reaction, Ostwald ripening,...

Mathematics Subject Classification 2000: 34C25, 34B16, 35R35

Departmento de Matematica Aplicada
University Complutense de Madrid
Postal address: Plaza de las Ciencias 3, 28040 Madrid
ildefonso.diaz@mat.ucm.es

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Maths and chemistry, a necessary relationship: A historical perspective and some current results from computational chemistry

Bernardo Herradón

Chemistry is the science that studies the composition, the structure, properties and transformations of matter; mainly at atomic and molecular levels.
By the end of 18th century, mostly initiated by the work of Lavoisier (1743-1794), the experimental work in chemistry was guided by the scientific method; which allowed obtaining accurate experimental data that, in turn, gave place to the fundamental quantitative laws of chemistry (Proust, Dalton, Gay-Lussac, Avogadro and Richter laws). By the first third of 19th century, a new chemical discipline was born: organic synthesis; that allowed chemists to make in a laboratory a multitude of chemical compounds, both natural and unnatural.
In this manner, chemistry provided human being with many of the goods necessary to have a more comfortable life: from chemicals to care our health up to materials to make clothes. This situation is still kept in the 21st century. Nowadays, chemistry is providing chemical substances to make materials that benefits our lives in such as diverse areas as energy, health, food, domestic stuffs, sports, leisure, and so on [1].
However, although the progress of chemistry, both theoretical and practical, have been impressive in the last two centuries; some fundamental concepts in chemistry need to be accurately defined, characterized and, when possible, measured. This goal is an objective of chemistry for the next decades; and it will be achieved through the *mathematization* of chemistry.
The relationship between chemistry and mathematics have been scarce along the history, and most of the times, this relation came through the work by physicists. In this talk, we will summarize the historical development of modern chemistry, especially in its close relationship with physics as well as the role that mathematics have had in this development; as well as the important role that mathematics will have in the future of chemistry. Some key interdisciplinary areas between chemistry and mathematics will be presented, both in its present status and potential future development.
The last part of the talk will deal with current developments in our group on computational chemistry, with applications on structural chemistry [2], on toxicology [3] and, especially, on aromaticity; where neural networks have proved as useful tools to classify organic molecules according to its aromaticity/non-aromaticity/antiaromaticity [4]. Further developments of this methodology have allowed to quantify this important property [5] as well as to establish structure-property relationships [6, 7] (Figure 1).

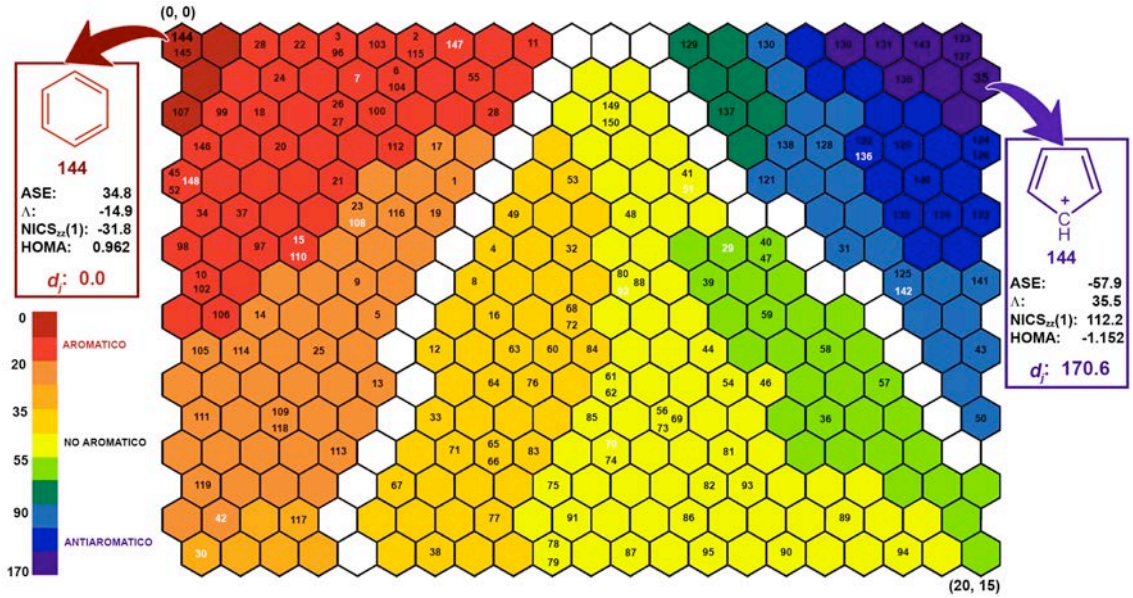

Figure 1. A neural network used to classify organic compounds according their character (aromatic, non-aromatic and antiaromatic). The Eucliden distance between neurons allows to quantify aromaticity/antiaromaticity.

Keywords: history of chemistry, mathematical influence on the development of chemistry, physics, computational chemistry, aromaticity, neural networks

Mathematics Subject Classification 2000: 81-08, 92E10, 92E99

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Instituto de Química Orgánica General
Consejo Superior de Investigaciones Científicas
Juan de la Cierva 3, 28006 Madrid
b.herradon@csic.es

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Two different mathematical contributions to chemistry: Special functions and Regression Models

Chelo Ferreira

We present two different examples about the relation between Chemistry and Mathematics. The first example deals with two expansions of the Randles-Sevcik function $\sqrt{\pi}\chi(x)$ (from electrochemistry). The second one provides a prediction model of wine aroma properties from aroma chemical composition.

Keywords: Randles-Sevcik function, asymptotic expansions, wine, aroma, PLS models.

Mathematics Subject Classification 2000: 41A60, 30E20, 62J05, 62J12

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Department of Applied Mathematics. IUMA
University of Zaragoza
cferrei@unizar.es

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Lattice Boltzmann solution of FENE constitutive equations for polymeric liquids

L. Bergamasco, **S. Izquierdo**,

The lattice Boltzmann method is a numerical approach based on kinetic theory for the solution of transport-phenomena equations. The computational efficiency and its kinetic origin makes it an attractive approach for a wide number of applications. With regards to polymeric liquids, it can be applied for solving material models described in the Fokker-Planck formalism, as it has been recently proved by [1]. Nonetheless, the computational issues concerned with the proposed approach have not yet been addressed. In the present work we aim to analyze the lattice Boltzmann solution of non-rigid dumbbell models with finitely extensible nonlinear elastic (FENE) potential. We will focus on the numerical issues concerned with the improvement of the computational efficiency, which include: reduced lattices, preconditioning and acceleration on graphic cards. In addition, the dimensionless limits for the numerical schemes proposed will be discussed, namely the acoustic and viscous limits for the Weissenberg number.

Keywords: Fokker-Planck, FENE dumbbell models, lattice Boltzmann method.

Mathematics Subject Classification 2000: 76A05, 76M12, 76M99

References

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Materials and Components
Instituto Tecnológico de Aragón (ITA)
María de Luna 8, 50018 Zaragoza, Spain
lbergamasco@ita.es, sizquierdo@ita.es

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Numerical simulation of the synthesis of iron nanoparticles prepared in a laser pyrolysis reactor

L. Usón*√, M. Arruebo*, M. Miana.**

A common way to synthesize Fe nanoparticles of 7 – 12 nm in diameter is by infrared laser decomposition of iron pentacarbonyl in an SF_6 gas stream ([1], [2]). Even though this laser-driven pyrolysis shows many advantages (i.e., continuous production, high throughput, etc.) it also has some drawbacks which need to be improved in order to avoid undesired nanoparticles agglomeration, polydispersity and material loss in the reactor walls. The aim of this work is the development of a CFD three dimensional numerical model to improve the physic-chemical characteristics of the resulting nanoparticles obtained in a laser pyrolysis rector by analyzing several operating conditions and reactor configurations.
A complete set of numerical models including multiphase fluid dynamics, laser heating, volumetric reaction and aerosol dynamics (with particle transport and evolution by convection, diffusion, nucleation, surface growth, coagulation and coalescence processes) must be solved by using ANSYS – FLUENT® software to perfectly describe the laser reactor. Thus, the project consists of four stages. First, non reacting isothermal fluid dynamics was studied to have an initial view of the fluid patterns inside the reactor. Next, heating and reaction phenomena have been studied in a simplified axisymmetric model. At this moment, the simplified axisymmetric model is being tuned to take into account particle formation from the heterogeneous reaction ([3], [4]). Finally, the population balance equation [5] will be applied to model the growth and coalescence of the nanoparticles as a function of the reactor configuration, inlet feeds, heat generation and vacuum pressure in the outlet.

Keywords: CFD, laser pyrolysis, iron nanoparticles, population balance equation.
Mathematics Subject Classification 2000: 76T25, 80A32, 76M12

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* Institute of Nanoscience of Aragón, University of Zaragoza. C/ Mariano Esquillor s/n, Zaragoza,
** Institute of Technology of Aragón, C/ María de Luna, nº 8, Zaragoza,
√ Corresponding author: 488635@unizar.es (L. Usón)

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Isomerization system LiCN/LiNC: Geometrodynamical version

Alberto Vergel[*1], **Juan Carlos Losada**[1], **Florentino Borondo**[2]
Rosa M. Benito[1]

We present a canonical approach to ascertain classical chaos in the dynamics of the title reaction, based on the use of an adequate language to deal with the stability problem for a general dynamical system.

Seeking for both simplicity and generality, we have adopted the geometrical focusing in order to rewrite the main settings, identifying the physical problem with a geometrical one in terms of abstract differential geometry.

For this purpose we apply the *Maupertuis' Principle*

$$\delta \int 2T dt = \delta \int \left(g_{ij}\dot{q}^i\dot{q}^j\right)^{\frac{1}{2}} dt = \delta \int ds = 0$$

with T = kinetical energy, g_{ij} = the *Jacobi's metric* [2] and s = arc-length parameter.

For a fixed energy level E, the dynamical information is fully coded in a Riemannian manifold (M_E, g) *(Mechanical manifold)* endowed with the *Jacobi's metric tensor* g

$$g \equiv g_{ij} = 2(E - V(q))a_{ij}(q)$$

where $a_{ij}(q)$ = mass matrix (kinetic energy) and $V(q)$ = potential energy

being the accesible region (Hill's region) $M_E = \{q \in M / V(q) \leq E\}$.

Geodesics of this *Mechanical manifold* correspond with the usual trajectories for the dynamical system.

Similarly, instability for trajectories corresponds to the geodesic separation, completely governed by the *Jacobi-Levi-Civita equation* via *Riemann-Christoffel* curvature tensor.

$$\frac{\nabla^2 J(s)}{ds^2} + R(\dot{\gamma}(s), J(s))\dot{\gamma}(s) = 0$$

with $\gamma(s)$ a normal geodesic, $\dot{\gamma} = \frac{d\gamma}{ds}$,

$J(s) \in T_{\gamma(s)}M$ the geodesic separation vector field, $\frac{\nabla}{ds}$ = covariant derivative.

$R(X,Y) = \nabla_X\nabla_Y - \nabla_Y\nabla_X - \nabla_{[X,Y]}$ the *Riemann-Christoffel curvature tensor*

We can identify physical variables with geometrical quantities as follows:

Dynamics		**Geometrý**
(Time)	$t \longleftrightarrow s$	(Arc-length)
(Potential)	$V \longleftrightarrow g_{ij}$	(Metric)
(Force)	$\partial V \longleftrightarrow \Gamma^i_{jk}$	(Christoffel's symbols)
(Conserved quantities)	$\longleftrightarrow$	(Simetries)
(Instability)	$\longleftrightarrow$	(Curvature)

As application to a realistic model, we show the order-chaos transition study for the isomerization system LiCN/LiNC[1] for two degrees of freedom.

This molecular system can be described through the Hamiltonian

$$H = \frac{P_R^2}{2\mu_1} + \frac{1}{2}\left(\frac{1}{\mu_1 R^2} + \frac{1}{\mu_2 r_e^2}\right) P_\theta^2 + V(R,\theta) \equiv \frac{1}{2} a^{ij} P_i P_j + V(R,\theta)$$

where R y θ represent Jacobi's coordinates describing the molecular system Li-CN and the distance C-N is fixed constant to its equilibrium value r_e.

We will show that the chaotic behaviour for the LiCN/LiNC system springs out with the appearing of convex parts in the border of the corresponding *Hill's region* i.e. $\partial M_E = \{q \in M_E / V(q) = E\}$ in a similar way to the *classical billards* or the *geometrical optics* in non homogeneous media.

Keywords: Jacobi metric, Curvature, Chaos, Isomerization reaction

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*alberto.vergel.otero@alumnos.upm.es

[1]Grupo de Sistemas Complejos y Departamento de Física y Mecánica,
Escuela Técnica Superior de Ingenieros Agrónomos
Universidad Politécnica de Madrid, E-28040 Madrid

[2]Departamento de Química, e Instituto de Ciencias Matemáticas CSIC-UAM-UC3M-UCM,
Universidad Autónoma de Madrid
Cantoblanco, E-28049 Madrid

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A modified Counter Current Back Mixing (CCBM) model to predict the solid axial mixing in a Two Section & Two Zone Fluidized Bed Reactor

Ignacio Julián, Javier Herguido[1], Miguel Menéndez[2]

The Two Section & Two Zone Fluidized Bed Reactor (TS-TZFBR) is a novel multipurpose reactor developed by the CREG research group (University of Zaragoza). This reactor integrates reaction and catalyst regeneration in a single vessel and becomes especially attractive to carry out heterogeneous catalytic reactions, where the catalyst suffers from a rapid loss of activity due to coke deposition over its surface [1]. The steady state operation is provided by the catalyst circulation between reactor zones. Therefore, the solids axial mixing determines the TS-TZFBR performance. Among the developed models to predict the particles circulation in fluidized beds, the Counter Current Back Mixing model (CCBM) has been largely used. The CCBM model is based on the three-phase system proposed by van Deemter (1961) [2]. This model depicts the bed as a multiple phase system with an upward flow of gas and wake phases and a downward flow in the dense phase. Solids exchange occurs between wake and emulsion phases. Mass balances over the individual phases are represented by a system of hyperbolic partial differential equations as a function of mixing time, t, and bed height, z. From this model, time and location variables can be uncoupled by applying the "kinematic model" proposed by Lakshmanan and Potter (1990) [3]. It consists in considering bed phases as divided into small compartments which move in instantaneous jumps, after spending some time exchanging solids with the adjacent phases. In this work, a kinematic solution of the CCBM model has been applied to predict the solid axial mixing in a Two Section & Two Zone Fluidized Bed Reactor (TS-TZFBR). The CCBM model parameters (u1, f1 and kw) have been related to the TS-TZFBR hydrodynamics and geometry, e.g. bubble size correlations, bed void fraction, gas velocity and transition section between bed zones. Experimental verification has been carried out using phosphorescent Eu-Dy/SrAl2O4 particles to measure the solids axial mixing between zones.

Department of Chemical Engineering and Environmental Technologies (IQTMA) University of Zaragoza Mariano Esquillor s/n, 50018 Zaragoza ijulian@unizar.es

Keywords: CCBM model, fluidized bed reactor, solid axial mixing

Mathematics Subject Classification 2000: 35L95

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Department of Chemical Engineering and Environmental Technologies (IQTMA)
University of Zaragoza
C/ Mariano Esquillor s/n, 50018 Zaragoza
ijulian@unizar.es

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Transition state theory: The phase space perspective

T. Uzer[1], **G. Haller**[2], **C. Jaffé**[3], **J.F. Palacián**[4], **P. Yanguas**[5]

Dynamical systems theory is used to construct a phase-space version of Transition State Theory. Special multidimensional separatrices are found which act as impenetrable barriers in phase space between trajectories that which lead to reactions and those which do not. The elusive momentum-dependent transition state between reactants and products is thereby characterized using a practical algorithm. The theory is applied to various examples of chemical reactions and atomic physics. In particular, the geometry of electron dynamics in the neighborhood of the rank-two saddle associated with the nonsequentual double ionization of helium is analyzed. As in the rank-one saddle case, codimension-one normally hyperbolic invariant manifolds turn out to control the rates of the correlated electron dynamics within each energy surface. The construction of these manifolds, however, is more involved here and requires the use of pseudo-hyperbolic invariant manifold theory. The work is based in the papers [1, 2].

Keywords: Rank-one and rank-n saddles, transition state theory, normally-hyperbolic invariant manifolds, pseudo-hyperbolic invariant structures, ionization of helium.

Mathematics Subject Classification 2000: 37C75, 37D10, 37J40, 70H09, 81V45, 78A35

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[1]Center for Nonlinear Sciences, School of Physics
Georgia Institute of Technology
Atlanta, GA, 30332-0430, USA
turgay.uzer@physics.gatech.edu

[2]Department of Mechanical Engineering and Department of Mathematics and Statistics
McGill University
Montreal, QC H3A 2K6, Canada
george.haller@mcgill.ca

[3]Department of Chemistry
West Virginia University
Morgantown, WV 26506-6045, USA
cjaffe@wvu.edu

[4]Departmento de Ingeniería Matemática e Informática
Universidad Pública de Navarra
31006, Pamplona, Spain
palacian@unavarra.es

[5]Departmento de Ingeniería Matemática e Informática
Universidad Pública de Navarra
31006, Pamplona, Spain
yanguas@unavarra.es

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Mathematical foundations of the transition state theory

J.F. Palacián[1], **G. Haller**[2], **C. Jaffé**[3], **T. Uzer**[4], **P. Yanguas**[5]

We present a comprehensive examination of the invariant structures associated with rank-one and higher-rank saddles. Codimension one normally hyperbolic invariant manifolds turn out to regulate transport and are the basic structures in the construction of the transition state. We build all the geometrical structures using (pseudo)-hyperbolic invariant and normal form theories. Rank-one saddles are more typical but higher-rank saddles occur in numerous contexts in celestial mechanics, chemical reactions and atomic physics. We present the main aspects of the theory from a dynamical systems perspective, focusing also on the practical implementation from which we choose our illustrative example. We choose the problem of the double ionization of helium in an external electric field to illustrate the theory. Our presentation is based in the paper [1].

Keywords: Rank-one and rank-n saddles, pseudo-hyperbolic invariant structures, normally-hyperbolic invariant manifolds, transition state theory.

Mathematics Subject Classification 2000: 37C75, 37D10, 37J40, 70H09, 81V45, 78A35

References

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[1]Departmento de Ingeniería Matemática e Informática
Universidad Pública de Navarra
31006, Pamplona, Spain
palacian@unavarra.es

[2]Department of Mechanical Engineering and Department of Mathematics and Statistics
McGill University
Montreal, QC H3A 2K6, Canada
george.haller@mcgill.ca

[3]Department of Chemistry
West Virginia University
Morgantown, WV 26506-6045, USA
cjaffe@wvu.edu

[4]Center for Nonlinear Sciences, School of Physics
Georgia Institute of Technology
Atlanta, GA, 30332-0430, USA
turgay.uzer@physics.gatech.edu

[5]Departmento de Ingeniería Matemática e Informática
Universidad Pública de Navarra
31006, Pamplona, Spain
yanguas@unavarra.es

Maths & Chemistry 2012
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Mathematics and Nanotechnology

Tim G. Myers, **Michelle M. McDevette**[1], **Francesc Font**[2]

Nanoscience has made great leaps forward in recent times, primarily through the experimental sciences such as chemistry and physics. The mathematics, which can be essential to an understanding of the basic processes, lags far behind.

In this talk we deal with three applications of mathematics to nanotechnology and show how at times relatively simple continuum theory can explain experimentally observed nanoscale phenomena.

1. Fast flow through carbon nanotubes – It has been well documented that the flow of water through carbon nanotubes is much greater than that predicted by classical flow theory, see [1]. A plausible explanation can be found by applying unidirectional flow theory in the presence of a *depletion* layer, which accounts for the hydrophobicity of the channel. The results match well with both experiment and molecular dynamics,

2. Melting of nanoparticles – As the radius of a melting nanoparticles decreases so does the rate of melting until in the final stages the particle seems to simply disappear[2]. However, standard mathematical theories indicate that melting is most rapid during the initial period. We will present a model that includes *melting point depression*, where the melt temperature decreases with curvature and in so doing find that the theoretical melting rate tends to infinity as the particle size tends to zero.

3. Nanofluid flow – Nanofluids are proposed as one of the most likely contenders for future heat removal requirements however, it is still not understood how they remove heat or indeed whether they really are better at heat removal than simpler fluids. This part of the talk will deal with the boundary layer flow of a nanofluid, showing how energy removal differs from that of the base fluid.

Keywords: Carbon nanotubes, flow enhancement, nanoparticle melting, phase change, melting point depression, nanofluids, heat transfer

Mathematics Subject Classification 2000: 82D80, 80A22, 76N20

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Centre de Recerca Matemàtica
Edifici C, Campus de Bellaterra
Barcelona 08193
tmyers@crm.cat

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A FEW MATHEMATICAL PROBLEMS INSPIRED BY CHEMISTRY

Miguel A. Herrero

ABSTRACT.- It is commonly acknowledged that the flourishing of Physics during the last centuries has been greatly favoured by its extensive use of mathematical methods. On the other hand, Mathematics has been deeply influenced by the many challenging problems that Physics has generated during that time. Such a mutually fruitful relationship has also been gradually developing with respect to other natural sciences. This fact has been instrumental in the outstanding growth of Biology, Chemistry, Geology and Medicine during the last century.

In this lecture I will review some examples of the interaction of Chemistry and Mathematics, paying attention to chemical problems which have had, and will have, a substantial impact in the development of whole mathematical areas. Such examples will include travelling wave solutions to reaction-diffusion systems, polymerization models as a tool to understand the formation of complex structures, and the controversial issue of the relation between morphology and biochemistry in the context of the origin of life on Earth.

Departamento de Matemática Aplicada
Facultad de Matemáticas, Universidad Complutense
28040 Madrid, Spain
Miguel_Herrero@mat.ucm.es.

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Model studies of electron transfer and conduction mediated by solitons in 1D and 2D crystal lattices

Manuel G. Velarde

First I shall present a model of soliton-like excitations in lattice chains/circuits/layers with units interacting with Morse interactions. Then, by adding external excess electrons, using the tight binding approximation (TBA), I shall show the formation of bound states between such charges and the soliton excitations, thus defining the "solectron" quasiparticle, in a sense that generalizes the (nowadays textbook) "polaron" concept of Landau, Pekar, Fröhlich, ... Adding Langevin stochastic sources to the mixed classical-quantum dynamics of the system, I shall illustrate the "long lasting" robustness and hence "practical" stability of the solectrons to moderate levels of heating (up to ambient temperature in biomolecules). The solectron moves in general with supersonic velocity though its actual velocity depends, e.g., on the strength of electron-lattice/phonon/soliton interaction. Possible applications of the theoretical predictions include a novel form of electron transfer (ET) in polymers like polydiacetylene (PDA and other derivative) crystals, synthetic DNA and biomolecules (trying to go beyond Marcus theory) and Ga-As or $LiNbO_3$(SiO) layers.

(For refs. cf: http://www.ucm.es/info/fluidos, Solectron theory papers)

Keywords: soliton, solectron, ET,DNA,...

Instituto Pluridisciplinar, Universidad Complutense de Madrid
Paseo Juan XXIII, 1, Madrid-28040
mgvelarde@pluri.ucm.es

Fundacion Universidad Alfonso X El Sabio
Villanueva de la Canada, Madrid-28691
mgvelarde@uax.es

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Mathematical Characterization of Chemical Reactions and Molecular Properties

Soledad Gutiérrez-Oliva, **Bárbara Herrera**, **Alejandro Toro-Labbé**

In this presentation we are going to review how mathematics helps characterize molecules and chemical reactions. The geometry and reactivity of molecular systems can be determined through the knowledge of their electronic structure which is, in turn, determined by solving the Schrödinger equation of quantum mechanics [1]. Interpretation of the information that comes out, a wave function characterizing the quantum state of the molecular probe, requires mathematical representations that allows to extract specific features and characterize the reactive behavior of molecules [2]. In this talk, special attention will be devoted to the mathematical representation of chemical reactivity descriptors and to the characterization of the mechanism of chemical reactions [3].

Keywords: Chemical Reactivity, Reaction Mechanisms.

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Laboratorio de Química Teórica Computacional (QTC),
Departmento de Química Física, Facultad de Química.
Pontificia Universidad Católica de Chile
Av. Vicuña Mackenna 4860, Santiago, Chile.
atola@puc.cl

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Combustion processes and cavitating bubble dynamics

Guillermo Hauke, **Cesar Dopazo**, **Daniel Fuster**[2]

A complete model for the radial solution of the Navier-Stokes equations in a spherical bubble surrounded by a liquid is used to investigate the combustion processes in vapor/air bubbles enriched with hydrogen. The numerical results provide new insights upon the effect of chemical reactions onto the bubble dynamics. Water evaporation/condensation is a fundamental transport phenomenon to estimate the dissociation reactions of water into OH. When implosions are intense enough, auto ignition conditions are firstly reached at the bubble center and a flame quickly propagates towards the interface. The coupling effects between the bubble dynamics and reaction process can produce internal shock waves which significantly increase the predicted temperatures and pressures inside the bubble [1, 2, 3].

Keywords: single bubble dynamics, cavitation, combustion

Mathematics Subject Classification 2000: 76-04, 76V05, 76M10, 76B10, 80A25

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Area de Mecanica de Fluidos
Escuela de Ingenieria y Arquitectura
C/Maria de Luna 3, 50018 Zaragoza Spain
ghauke@unizar.es
dopazo@unizar.es

[2]CNRS
UMR 7190, Institut Jean Le Rond d'Alembert, F-75005 Paris, FRANCE
fuster@dalembert.upmc.fr

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LIST OF PARTICIPANTS

- Turgay Uzer, (Georgia Tech, School of Physics of Atlanta)
- Herschel A. Räbitz, (Univ. of Princeton)
- Alejandro Toro-Labbé, Univ. Católica de Chile)
- Miguel Ángel Herrero, (Univ. Complutense de Madrid)
- Jesús Palacián, (Univ. Pública de Navarra)
- Tim Myers, (Centre de Recerca Matemàtica)
- Jesús Ildefonso Díaz, (Univ. Complutense de Madrid)
- Bernardo Herradón, (CSIC)
- Manuel García Velarde, (Univ. Complutense de Madrid)
- Manuel Calvo (Univ. of Zaragoza)
- Chelo Ferreira (Univ. of Zaragoza)
- Antonio Elipe (CUD)
- Juan I. Montijano (Univ. of Zaragoza)
- Tomás Grande (Univ. of Zaragoza)
- María Cruz López de Silanes (Univ. of Zaragoza)
- Flora Sayas (Univ. Pub. of Navarra)
- Ignacio Julián (Univ. of Zaragoza)
- Francisco Gaspar (Univ. of Zaragoza)
- José E. Galé (Univ. of Zaragoza)
- Francisco Lisbona (Univ. of Zaragoza)
- Luca Bergamasco (ITA)
- Natalia Romero (Univ. of La Rioja)
- Juan Manuel Peña (Univ. of Zaragoza)
- José Luis Gracia (Univ. of Zaragoza)
- Alberto Vergel, (Univ. Politécnica de Madrid)
- Jorge Ortigas (CUD)
- Inmaculada Gómez (Univ. of Zaragoza)
- Jesús Anzano (Univ. of Zaragoza)
- José María Franco (Univ. of Zaragoza)
- Manuel Alfaro (Univ. of Zaragoza)
- Pedro J. Miana (Univ. of Zaragoza)
- Luis Sánchez Lajusticia (Univ. of Zaragoza)
- Julio Bernués (Univ. of Zaragoza)
- Luis Rández (Univ. of Zaragoza)
- Natalia Boal (Univ. of Zaragoza)
- Laura Usón (INA)
- Patricia Yanguas (Univ. Pub. of Navarra)
- Daniel Casanova (Univ. of Zaragoza)
- Elvis Lacruz (Univ. of Zaragoza)
- Diego Izquierdo (Univ. of Zaragoza)
- Carmelo Clavero (Univ. of Zaragoza)
- Eduardo Martinez (Univ. of Zaragoza)