

**Consegna Premi INdAM-SIMAI 2012**

**Giornata di Studio "Prospettive di sviluppo della  
matematica applicata in Italia 2013"**

**LIBRO DEGLI ABSTRACTS**

**Aula Marconi, CNR -- Roma**

**11 Marzo 2013**





## **Vincitori del Premio INdAM-SIMAI 2012**



## Two-Phase and Micro-Macro Descriptions of Traffic Flow

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### Abstract

We present two frameworks for the description of traffic, both consisting in the coupling of systems of different types. First, we consider the 2-phase model [1, 3], where a scalar conservation law is coupled with a  $2 \times 2$  system. Then, we present the coupling of a micro- and a macroscopic models, the former consisting in a system of ordinary differential equations and the latter in the usual LWR conservation law, see [2, 4]. A comparison between the two different frameworks is also provided.

*Keywords:* hyperbolic systems of conservation laws; 2-phase traffic models; microscopic traffic flow models.

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Design of silicon based integrated optical devices  
using the finite element method

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## Abstract

Over the last decades, the request of larger bandwidth and faster communication has strongly pushed the photonics technology. Among the several components required in photonic integrated circuits, straight waveguides and small footprint ring resonators play a key role for many applications and require sophisticated electromagnetic analysis and design.

In the thesis, I have studied and optimized a full vectorial modal analysis based on the finite element method for lossless waveguides and ring resonators, using cartesian and cylindrical coordinate systems, respectively. After having computed the Rayleigh-Ritz functional for the non-self-adjoint case, a fully real formulation has been derived considering isotropic, anisotropic and magneto-optical materials. Using the node-based approach, the penalty function has been introduced to remove the spurious solutions [1]. Although its use is well-known for waveguides analysis, it has been introduced for the first time in ring resonator case. Finally, the  $\gamma$ -formulation, where the frequency is provided as input parameter and the propagation constant is the output eigenvalue, has been derived and effectively implemented avoiding the time-consuming iterations necessary in previous formulations [2]. After developing and validating the method on some examples, it has been employed to design two fundamental components for the integrated silicon photonics: laser sources [3, 4, 5] and isolators [6, 7, 8].

*Keywords:* Maxwell's equations, Finite element method.

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## Mesoscopic description of boundary effects in nanoscale heat transport

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### Abstract

The phonon-wall interactions play a central role in heat conduction in nanodevices, due to the small size of these systems. In macroscopic systems the influence of the boundary on the heat flow is restricted only to the so-called Knudsen layer, namely, a thin layer near the walls of the system, whose characteristic width is of the order of the mean-free path of the heat carriers. Far from the walls, the boundary conditions are not felt. In nanosystems, instead, since the characteristic size of the transversal section is smaller than (or at least comparable to) the mean-free path of the phonons (which are the main responsible of the heat transport), the boundary effects are felt everywhere in the system, and strongly influence the propagation of heat flow [1, 2]. In order to study the influence of the phonon-wall interactions on the longitudinal thermal conductivity in nanosystems, we use the phonon hydrodynamics complemented with boundary conditions for smooth and rough boundaries [3]. The dependence of the boundary conditions on the temperature of the system is analyzed as well. Several comparisons between our theoretical models and experimental data are made.

*Keywords:* phonon hydrodynamics, boundary conditions, silicon nanowires, thermal conductivity, rough surfaces, backscattering

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## A robust solver for stratified creeping flows

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### Abstract

The simulation of sedimentary basins on a geologic time scale calls for the solution of the movement of stratified fluids in the Stokes regime, see [1], [2]. This is an evolution problem and requires a robust three dimensional solver whose runs could last several hours or even days. Three main key areas have been identified: the multi-scale modeling, the implicit tracking of multi fluid flows and the preconditioning techniques. While the first area is a relatively straightforward application of the volume averaging technique, the other issues require a specific treatment. The tracking method should be conservative, robust and it should treat a number of fluids. Usually only the two fluid case is treated. This problem has been tackled in [3]. The conditioning number is the other main issue: the fact the various sedimentary layers that constitute the sedimentary basin have very different mechanical characteristics causes a bad conditioning of the Stokes problem. An efficient technique has been analyzed in [4] and the full algorithm is described [5]. The complete algorithm includes some other features such as the possibility of considering the movement of the basement of the basin and the effects of faults. A few references on how these techniques are useful also in very different fields, arising from the plasma physics, are included.

*Keywords: Level Set, Conditioning, Stokes problem, Computational geology*

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## **Contributi**



## Multivariate approximation on unstructured data with applications to real life cases

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### Abstract

In this contribution we present efficient algorithms for interpolating a large number of unstructured data on plane and spherical domains. These procedures are based on the partition of unity method, which is obtained locally combining radial basis functions and Shepard-type weight functions [4, 5]. The main goal of this work consists in constructing new and fast searching techniques in the localization of the nearest neighbor nodes, exploiting a suitable and optimal partition of the domain in cells. This approach, which strictly depends on the size of its subdomains, is obtained by connecting the method itself with the considered searching procedures, thus producing better efficiency than the ones in [1, 2, 3]. Numerical experiments show good performances of such algorithms, also considering some applications to Earth’s topography and geomagnetic data.

*Keywords:* partition of unity methods, fast searching procedures, scattered data interpolation, radial basis functions

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## Scaling laws for droplets spreading under contact line friction

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### Abstract

This talk is concerned with the spreading of a liquid droplet on a plane solid surface in the regime of lubrication approximation. The focus is on effective conditions which relate the speed of the contact line (where liquid, solid and vapor meet) to the microscopic contact angle. One such condition has been recently proposed by Weiqing Ren and Weinan E [1] : it includes into the model the effect of frictional forces which arise at the contact line from unbalanced components of the Young's stress, leading to an additional dissipation term in the energy balance. For speed-dependent contact angle conditions of rather general form, a matched asymptotic study is worked out, relating the macroscopic contact angle to the speed of the contact line. Here, well-posedness for a class of traveling- wave solutions, which does not seem to have been observed so far, is proved and used. For the specific model of Ren and E, ODE arguments are then applied to infer the intermediate scaling laws and their timescales of validity: in complete wetting, they depend crucially on the relative strength of surface friction (at the liquid-solid interface) versus contact-line friction; in partial wetting, they also depend on the magnitude of the static contact-angle. The results have been obtained jointly with Lorenzo Giacomelli (Sapienza University of Rome) [2].

*Keywords:* Moving contact line, droplets, thin film equations, fourth order degenerate parabolic equations, free boundary problems, lubrication theory, matched asymptotic expansions, intermediate scaling laws

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**Numerical simulation for 3D fractional diffusion equations  
to describe anomalous diffusion in porous media**

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## **Abstract**

The numerical simulation of fractional diffusion equations in three dimensions is considered, to describe fluid flow through porous media. A fractional version of the Alternating Direction Implicit (ADI) scheme is proposed. A strategy improving the speed of convergence by an extrapolation method is also presented. Both, homogeneous and heterogeneous media with a number of different characteristic particle size were considered. A number of numerical experiments simulating laboratory tests have been performed. Numerical results are given to support our theoretical analysis.

*Keywords:* anomalous diffusion; fractional diffusion, fractional partial derivatives; Alternating Direction Implicit (ADI) scheme; extrapolation techniques; experimental data.

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## Abstract

The theory of hysteresis operators developed in the recent years has proved to be a powerful tool for solving mathematical problems in various branches of applications, such as solid mechanics, material fatigue, ferromagnetism, phase transitions.

In a series of recent papers [1], [2], [3] we developed a model for thermo-elasto-plastic oscillations of beams and plates with hysteresis and material fatigue. It is well known that plastic deformations lead to energy dissipation and material fatigue, which is in turn manifested by material softening, heat release and material failure in finite time. In view of engineering applications, it is relevant to account also for the possibility of having decreasing fatigue rate, so that the material can be partially repaired by local melting.

A way to achieve this goal can be to account also for phase transitions in the model, so that the time of failure of the material can be shifted and, possibly considering a sufficiently large time interval of observation, a global solution of the corresponding PDEs system can be found.

In this talk we discuss thermodynamical consistency of the new model including together with the fatigue parameter, also a new parameter of phase transition that describes the degree of melting of the material, and outline some new perspectives and related mathematical results.

*Keywords:* hysteresis, phase transitions, elastoplasticity, material fatigue

## References

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**The energy based method applied  
to the damped wave equation**

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## **Abstract**

The study of wave propagation modeled by partial differential equations of hyperbolic type and by systems of boundary integral equations (BIEs) is important in many physic and engineering problems. Of particular interest is the analysis of damping phenomena that occur, for example, in fluid dynamics, in kinetic theory and semiconductors: the dissipation is generated in the interaction of the waves with the propagation medium and can be also closely related to the dispersion, as in the interactions between water streams and surface waves or in ferromagnetic materials. For the numerical solution of these problems, we need consistent approximations and accurate simulations even on large time intervals. For the damped wave equation, consider the extension of the “energetic” weak formulation, conceived by the Numerical Analysis Group at the University of Parma and introduced during the previous edition of this SIMAI conference for the undamped wave equation.

This new weak formulation, based on the energy identity satisfied by any solution of the scalar wave problem, was presented and applied to retarded BIEs related to the wave equation without damping terms, directly expressed in the space-time domain with proof of important stability properties in time and achieving, by Boundary Element Method (BEM), significant numerical results.

The advantages of BEM, when compared to domain methods, are well known, particularly in presence of unbounded domains, however, for example, the presence of volume forces in small portions of the whole definition domain of the problem makes the coupling with finite element methods (FEM) advantageous.

Now, first results for problems modeled by 1D damped wave equation have been obtained with BEM-FEM coupling combined with the extension of the “energetic” weak formulation, in bounded and unbounded multi-domains, and here they will be presented and discussed.

*Keywords:* wave equation, damping, “energetic” Galerkin boundary element method.

## Exponentially-fitted quadrature methods for evolution problems with periodic solution

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### Abstract

The interest for numerical solution of physical and biological problems with oscillating and/or periodic behaviour requires the use of special-purpose methods. Examples include the electromagnetic scattering, the response of nonlinear circuits to a periodic input and the evolution of an age-structured population. These problems are characterized by either infinite integrals of type:

$$\int_0^{\infty} e^{-x} f(x) dx \quad (1)$$

where  $f$  is oscillatory function, or by Volterra integral equations of type:

$$\begin{aligned} y(x) &= f(x) + \int_{-\infty}^x k(x-s)y(s)ds, & x \in [0, X] \\ y(x) &= \psi(x), & x \leq 0, \end{aligned} \quad (2)$$

where one assumes  $y$  being a periodic solution. By exploiting the Exponential Fitting theory [1, 2, 3, 4, 5], a new class of quadrature rules, that are a generalization of the usual Gauss-Laguerre formulae, for problem (1) and a new direct quadrature (DQ) method for problem (2) are derived, respectively. Two extra problems appear in the context of building the exponentially-fitted (*ef*) DQ method. The first one is the construction of a two-nodes *ef* quadrature rule of Gaussian type, that is a generalization of the usual two-nodes Gauss-Legendre formula, on which the DQ method is based. The second problem is the building of a suitable *ef* interpolation technique on four points which preserves the order of convergence of the overall method. These works are in collaboration with L. Gr. Ixaru (National Institute of Physics and Nuclear Engineering, Bucharest, Romania), B. Paternoster, A. Cardone and D. Conte (University of Salerno).

**Keywords:** Exponential fitting, Periodic, Infinite integral, Volterra integral equations.

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**Mathematical Desk for Italian Industry  
Sportello Matematico per l'Industria Italiana**

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## **Abstract**

Mathematical Desk for Italian Industry is the english translation for the italian applied and industrial research project SMII, namely, Sportello Matematico per l'Industria Italiana. The SMII project is established in Rome at the "Istituto per le Applicazioni del Calcolo Mauro Picone" (IAC), an institute of the Italian National Research Council (CNR), and has been funded by the Italian Ministry for Education and Research (MIUR) for a starting period of three years. Its activities are organized in coordination with the Italian Society of Applied and Industrial Mathematics (SIMAI) and the Italian Association of Operations Research (AIRO). The mission of the Mathematical Desk for Italian Industry is that of building a concrete bridge of common interests between the italian scientific community of applied mathematics and the world of the italian enterprises, focused on the development of industrial research projects and innovation. The main objective of the SMII is to realize an effective and qualified intermediation role in the field of scientific and technological transfer, based in particular on the role of mathematics. This way, the SMII project aims to encourage italian enterprises to improve the quality of their products and processes through the adoption of mathematical methods developed ad-hoc for their needs, thanks to a fruitful cooperation with a network of italian excellence centers of industrial mathematics. Additional objectives of the SMII project are: to give more visibility to what mathematics can offer to industry; to create an Italian network of excellence in industrial mathematics, possibly in an international context of European networks; to stimulate future engagement of young mathematicians in industry, creating a natural network of contacts between advanced academic research in mathematics and industrial research.

Started in December 2012, the SMII project is currently developed by a team of four researchers working at the IAC in Rome. The research team is supervised by the scientific and institutional direction of IAC-CNR, and is assisted by an Advisory Board, that includes several major italian experts on Applied and Industrial Mathematics. More information on SMII project is available on the website [www.sportellomatematico.it](http://www.sportellomatematico.it) where enterprises can apply directly to ask for consultancies in order to start developing innovation projects in the field of applied and industrial mathematics.

*Keywords:* Applied mathematics, Industrial research, Technology transfer, Project management, Networking

## **Buchberger graphs**

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## **Abstract**

The Buchberger graph arises from the combinatorial nature of some algebraic objects: the monomial ideals ([1]). Since the Buchberger graph  $G$  of a monomial ideal  $I$  in three variables can be nicely embedded into the staircase diagram of  $I$ ,  $G$  can be visualized in  $\mathbf{R}^3$  and can be easily studied (connectedness, planarity, ...).

We study the Buchberger graph of classes of monomial ideals in three variables in order to find applications in different fields. In general, one uses combinatorial and geometric techniques to study data associated to phenomena, being the data a lattice points set  $D$  contained in  $\mathbf{N}^3$ . In particular, we apply the method to study data that are very regular and to connect them by the paths of the Buchberger graph associated to a monomial ideal whose generators are constructed by the set  $D$ .

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