InSPIRES: a science shop project

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A science shop is a methodology in which the universities and research centres allow citizens and civil organisations to raising questions, present problems and issues on any topic, according with the available expertise. The answer may require a simple bibliographic consultation or a specific investigation. In any case, the research is assigned to students as part of their work for an exam or as the final dissertation, under the supervision of an experienced researcher. The InSPIRES project aims at favouring the birth of new science shops, especially in the south Europe and related countries, extract the best practices and experimenting with more participative methodologies. We shall illustrate some examples of existing science shops and the planned workflow for the University of Florence.
Accurate quantum chemical protocols for the determination of structural, spectroscopic and energetic properties of small and medium size molecular systems of biochemical interest

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Retrieving molecular structures is one of the principal concerns in many areas of chemistry, and the last decades have seen many efforts to determine accurate molecular geometries for systems of increasing size and complexity. Nowadays, this represents one of the main approaches to understand the structure of biochemical molecules, because of the close relation between molecular structure and functionality. In this context, rotational spectroscopy provides very accurate experimental information on the geometry of molecules in the gas phase, thus avoiding the complications arising from environmental effects in tuning the overall conformational behavior. Comparing this kind of data with those obtained from the condensed phase allows one to discriminate between the inter- and intra- molecular interactions. However, the interpretation of rotational spectra is often a difficult task, hence laboratory experiments are strongly supported by quantum chemical calculations carried out by using suitable computational protocols to achieve the required accuracy. Theoretical spectroscopic parameters are then employed to assist and guide the interpretation of the experimental spectra. In order to accurately predict spectroscopic data, the harmonic force field should be computed at a suitable level of theory and then it is necessary to go beyond the harmonic approximation. For the purpose, the coupled cluster theory with singles, doubles excitations and a perturbative estimate of connected triples, CCSD(T), coupled to large basis sets has become the gold standard for the accurate prediction of thermochemical and spectroscopic properties of small molecules. Even more accurate results, rivaling the most refined experimental techniques, can be obtained employing composite schemes [1]. In particular, in the "cheap" computational protocol, developed to handle small bio-molecules, the CCSD(T)/cc-pVTZ level of theory is considered as the starting point, while missing contributions (e.g. basis set extrapolation, higher excitations, core correlation effects) are recovered by employing second-order Møller–Plesset perturbation theory [2]. Anharmonic effects on structural, rotational and vibrational properties are then evaluated by density functional theory (DFT), specifically at B2PLYP/m-aug-cc-pVTZ-dH and B3LYP/SNSD levels.

In this work, quantum chemical calculations exploiting the "cheap" computational protocol and DFT methods are performed for accurately determining the structural and rotational-vibrational spectroscopic properties of L-threonine, creatinine, D-cycloserine and methanimidic acid.

References
Small group students activity: a mathematical model for improve the dynamics

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Nowadays active learning have gained more and more attention since such a methodology allows to improve the student learning [1]. In particular, the flipped classroom and the group work activities in classroom are one of the most used form of active learning [2], because during such activities the students act, interact and communicate much more than in usual frontal lessons settings [3]. In such a context, it is crucial to understand what are the variables which govern the student dynamics and even what is the role of the teacher during a small group activity. Thus, on the path of recent mathematical model of multi-agents dynamics and opinion dynamics [3, 4], Brunetto et al. [5] proposed a mathematical model for small group work activities exploiting the opinion dynamics model [6] and the theoretical framework “I can”-”You can” introduced by Andrà et al. [7], moreover the teacher has a crucial role in group work activities. This work, based on [8], deals with the control problem of multi-agent systems, when the agents are students who are asked to solve a mathematical task working in small group. The leader of the group is represented by the teacher who is allowed to make mathematical intervention during the students' activity with the purpose of improving students’ performance. Hence, the teacher opinion is the control variable of the dynamics which evolves to achieve some goals abstracted by an object function. To show the reliability of the model and the strategy of intervention of the teacher, we provide several numerical results and compare them with realistic scenarios.

More precisely, let \( N \) be the number of students whose opinions are abstracted by variables \( x_i, i=1,\ldots,N \), while \( x_{N+1} \) represents the opinion of the teacher and \( x_0 \) is the correct solution to the assigned math task. The dynamics of the group is described by a set of ordinary differential equations (e.g. see [6]) with suitable non-linear weights depending on the attitude of the students and their mathematical knowledge. In such a context, the teacher is supposed to act a strategy in order to minimize a suitable object function \( J \) which is designed to improve the students performance.

References

This talk proposes a systems approach to the theory of perception and learning in populations composed of many living entities. Starting from a phenomenological description of these processes, a mathematical structure is derived which is deemed to incorporate their complexity feature. The modeling is based on a generalization of kinetic theory methods where interactions are described by theoretical tools of game theory.

References


Learning by message-passing in networks of discrete synapses: the traffic congestion prediction

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Abstract

Belief Propagation (BP) is an iterative message passing algorithm that can be used to derive marginal probabilities on a system within the Bethe-Peierls approximation. It is not well understood how this deep learning method is able to learn and how it doesn’t get trapped in configurations with low computational performance. Since we aim to classify the congestion situations, we analyze the fundamental diagram of traffic which gives a relation between the traffic flow and the traffic density. A traffic congestion occurs when the density of the road grows up and the flow decreases. In order to predict congestion situations, we train the BP neural network using binarized vectors obtained by the processing of the fundamental diagram. We apply our method to real data which have been recorded by traffic detectors provided by Emilia Romagna region.

References


Nonlinear diffusion in material tissues:

a free boundary problem

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A free boundary problem on a finite interval is formulated and solved for a nonlinear diffusion-convection equation. The model is suitable to describe drug diffusion in arterial tissues after the drug is released by an arterial stent. The problem is reduced to a system of nonlinear integral equations, admitting a unique solution for small time. The existence of an exact solution corresponding to a moving front is also shown.

References


The UV-Vis spectral properties of aromatic amino acids can be exploited to probe protein structure, dynamics and interactions. In particular, Tyrosine (Tyr) spectroscopy is routinely used for studying proteins response to environmental changes. Tyrosine’s phenolic side chain (the \textit{p}-Cresol) is highly sensitive to its molecular environment thus making Tyr spectroscopy an appropriate choice for such a purpose. In this regard, a detailed understanding of the environmental effects on the chromophore electronic properties is highly important [1].

In this study, we theoretically reproduce the UV-Vis absorption spectrum of aqueous solutions of \textit{p}-Cresol, and zwitterionic, cationic and anionic Tyrosines, pinpointing the effects of the backbone protonation on the electronic absorption properties of the chromophore. To this purpose, we apply the Perturbed Matrix Method (PMM). The PMM is a method based on the first principles of Quantum Mechanics which permits to include the effects of the environment in the evaluation of the quantum properties of a quantum center (i.e. the system subpart to be treated at quantum mechanical level). The method was developed by Amadei et al. [2] and recently implemented in the Gaussian package with several improvements [3]. Molecular Dynamics (MD) simulations provided the statistical-mechanical ensemble for the study. To achieve a better accuracy in the MD sampling, the Force Field (FF) was parameterized \textit{ad hoc} for each solute of interest, deriving all the FF parameters according to the procedure implemented in JOYCE software [4].

References
A novel statistical procedure has been developed to optimize the parameters of a theoretical model through a supervised training process. The method exploits the combination of the linear ridge regression and the cross-validation techniques [1] with the differential evolution algorithm [2]. Both linear and non-linear parameters can be optimized, allowing the optimization of a wide variety of functional forms of the model. The procedure has been applied to the parametrization of non-bonded force fields of metal ions in soft matter, using as output references \textit{ab initio} forces and energies calculated for model systems. The methodology has been tested by generating the force fields of five metal ions (Zn$^{2+}$, Ni$^{2+}$, Mg$^{2+}$, Ca$^{2+}$, and Na$^+$) in water. The estimates of the thermodynamic and structural properties calculated from molecular dynamics simulations using our force fields are on average of better quality of the state of art level [3].

References


In this talk I will survey some recent advances in the statistical modelling of networks and I will discuss their application in the financial domain. I will consider the interbank market and I show how a suitable Stochastic Block Model can be used to identify the large scale (for example core-periphery) structure of the network. I then consider the dynamics of a network, proposing a statistical time series model able to capture the interplay between link temporal persistence and the memory properties of the nodes fitness. Finally, by using the Maximum Entropy principle, I will propose a method for reconstructing a bipartite network from partial information, showing that this method is very effective in estimating the systemic risk due to fire sale spillovers and portfolio overlaps among banks.
Computational methods such as Molecular Dynamics (MD) are powerful tools to estimate macroscopic properties from microscopic models [1]. These methodologies have shown to be especially useful to investigate the structure of organic liquids that are used as solvents in chemical, biological, and technological sectors. In classical MD, electronic degrees of freedom are replaced by a simplified set of functions called Force Field (FF) in order to make atomistic simulations computationally feasible. FFs are usually trained on the basis of higher level (quantum mechanical) calculations and/or experimental data. The selection and the availability of the most appropriate FF for the system to be investigated is crucial for the reliability of the simulation results. Another critical aspect in FFs is the electrostatic interactions based on the generation of partial charges. Several strategies have been followed to determine appropriate partial atomic charges, one of them is to optimize their values to reproduce the QM derived electrostatic potential surrounding a molecule [2]. The atomic charges values depend strongly on the level of theory used in QM calculation and the description of solvation effects.

Here, we present a FFs development method for different classes of molecules with minimal use of empiric parameters and able to reproduce experimental values of target properties and to explain accurately their microscopic liquid structure.

One studied molecular class is formed by flexible molecules which requires dihedral angles parameterization, essential to describe conformational equilibrium [3]. Another class consists of aromatic molecules, for which a new protocol for point charges fitting has been developed [4]. The new FFs has been applied to perform MD simulations of pure liquids as well solutions. Bulk properties and an accurate nanoscopic description have been derived and compared with experimental data.

References
Recent results about the Mercedes-Benz water model

The Mercedes-Benz model of water is a simple two-dimensional model that can reproduce some of the anomalies of water, in particular the decrease of density of ice with respect to liquid water. We describe the lattice version of the model and discuss its phase diagram with respect to the variation of some parameters. We also show how to reproduce the phenomenon of supercooled water and the eutectic effect of salt and ice mixtures.
Hydrogen Bond Dynamics of Imidazole in Water

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Imidazole is an aromatic heterocycle with a 5-membered ring, as shown in Figure 1. The imidazole ring occurs, as molecule or building block, in systems with important biological, pharmacological and chemical applications [1,2]. In water, at physiological pH, imidazole is present both as neutral and protonated species and interacts with this solvent forming hydrogen bonds [2]. To characterize the structural and dynamic properties of imidazole in water, ab initio molecular dynamics simulations have been performed with the Car-Parrinello method (CPMD) [3]. During these simulations, the potential is determined within the framework of density functional theory, whereas the van der Waals interactions have been properly considered with the Grimme method [4]. Since CPMD simulations provide a description of the hydrogen bond interactions in agreement with experimental findings [2], selected results have been adopted to validate a series of force fields for classical molecular dynamics simulations. Accurate force fields are needed to determine structural and dynamic properties of imidazole in aqueous solution for a correct interpretation of the experimental measurements.

Figure 1. Molecular structure of imidazole. Atom colors: carbon, grey; nitrogen, blue; hydrogen, white.

References
A Rare Mutation Model in a Spatial Heterogeneous Environment

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We propose a stochastic model in evolutionary game theory where individuals (or subpopulations) can mutate changing their strategies randomly (but rarely) and explore the external environment. This environment affects the selective pressure by modifying the payoff arising from the interactions between strategies. We derive a Fokker-Plank integro-differential equation and provide Monte Carlo simulations for the Hawks vs Doves game. In particular we show that, in some cases, taking into account the external environment favors the persistence of the low-fitness strategy.

Evolutionary Dynamics describes biological systems subject to Darwinian Evolution by taking into account the main mechanisms and phenomena of Evolution itself. In [2], Maynard Smith and Price propose an instance of this approach by considering a population modified according to the replicator dynamics, a system of differential equations describing the selection and adaptation mechanism.

The rate of increment of a type is given by its absolute fitness, balanced with the average fitness of the population. In evolutionary matrix game theory the vector of absolute fitness is defined by means of a matrix of payoff that rules the interplay between different strategists.

However, it is clear that the basic element for the generation of evolutionary novelties are mutations. The quasispecies equation, dating back to the 1970s, modifies the growth rate of each species by considering the dispersion due to the birth of mutated offspring. However, an important aspect of mutations stands in their randomness, which is quite underrated in the quasispecies equation. Since then many more refined models have been proposed to put into the right light randomness; we refer at [1], where it has been proposed a macroscopic stochastic model where mutations occur at a different time scale than selection.

Within the framework of social dilemma, where the types are read as strategies, a "mutation" happens when a player changes his strategy. The model in [1] assumes that such events happen on rare and random occasions, even more than once before the system reaches its stable state.

In this paper we take a step further and address our attention to the environment, seen as a place where individuals can evolve but also as a factor that can influence the dynamics of interaction between strategists. The model takes into account how the natural environment can modify the interactions between individuals, changing selective pressures; we add a new variable that stands for the position of the population or, more widely, for an external parameter that affects the results of the interplay between strategies. It changes according to a velocity, partly deterministic, partly stochastic, and influences the selection mechanism because the payoff matrix depends on y. In some particular cases, the environment itself allows for the survival of the low fitness species.

References


Mean field coarse-graining of confined fluids

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Nowadays, multiscale modelling techniques hold great promise for the representation of physical systems in relatively broad spatial and temporal scales. Such procedures involve the combination of different computational tools describing the same system at different resolutions. Reaching larger scales often requires performing a coarse-graining procedure in order to obtain a simpler but more computationally efficient model.

At a coarse-grained level, stochastic models are very often used to address the problem of modelling of adsorption and diffusion of fluids in microporous materials. In order to represent accurately thermodynamic properties, such as the average local density as a function of the fugacity, it is crucial to estimate correctly the amount of free energy associated with each local configuration of the coarse-grained degrees of freedom. For this purpose, Tunca and Ford proposed a Monte Carlo approach based on the Expanded Ensemble Method to calculate the partition function of an isolated pair of connected pores [1]. In this work, we introduce a new protocol to obtain a coarse-grained model by employing a mean field approximation of the pore lattice. In this procedure, instead of considering isolated pores and isolated pair of connected pores, the first neighborhood is included as a set of fictitious, mean field, pores, which imitates the same topology of the reference system. This method allows including first neighbors contributions to single-cell and pair partition functions estimates.

For the sake of comparison between the two approaches, we chosen to use a simple lattice gas model as a common reference system. Such models are commonly used to simulate fluid adsorption and diffusion in a certain environment, from a molecular point of view [2]. Due to the discrete nature of lattice models, local partition functions can be calculated exactly, producing a flawless reference for the comparison purpose.

The reference lattice is a grid of sites, each able to host one molecule at most, and its global state is defined by the set of occupancies of all the sites. In the coarse-grained version of such system, the lattice is uniformly partitioned into non-overlapping cells, each containing the same number of sites, and the state of the coarse-grained system is defined as the set of cell (rather than site) occupancies.

The effective occupancy dependent free energy of single cells and cell pairs are estimated through recurrence relations, implying precise mean field models of the cell lattice. Local free energies are supposed to depend on temperature but not on the fugacity (or chemical potential). Finally, the system is simulated via a Metropolis-Hastings scheme. This model is capable of accurately reproduce reference system static properties such as the average occupancy and local density fluctuations.

References


Exploiting network knowledge for biomedical application

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Network are ubiquitous in nature, and particularly in biology, due to the strong interacting nature of its elements (cells, genes, proteins, metabolites).

In this presentation we will give an overview of which biological data can be used for this approaches, and which biological datasets can be exploited which already show a network structure.

A case study on real data will be shown, that combines multiple biological and clinical data from public databases for developing new multidrug treatments or perform trans-tumour drug translation in oncology.
Kinetic and Multiscale Models of Traffic Flows

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In this talk we present a modelling approach to multi-agent systems, with special reference to vehicular and pedestrian traffic, based on Boltzmann-type kinetic equations and measure-valued conservation laws. We discuss how to pass from microscopic binary interactions to the description of emerging collective trends by means of probabilistic and multiscale representations of the particle system. In particular, we show that hyperbolic equations with non-local flux accounting for interactive dynamics arise as a natural modelling paradigm in such a context under a suitable scaling of the kinetic equations.

References

Opinion dynamics over kinetic networks

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In recent years the importance of large scale social networks has grown enormously due to the rapid proliferation of novel communication platforms. The need to handle with millions, and often billions, of vertices implies a considerable shift of interest to large-scale statistical properties of networks which may be described through the methods of the kinetic theory. In this talk we propose a kinetic description of the agents' distribution over the evolving network which combines an opinion update based on binary interactions between agents with a dynamic creation and removal process of new connections [1,2,3]. The number of connections of each agent influences the spreading of opinions in the network, further the way connections are created is influenced by the agents' opinion. We will study the evolution of the network of connections by showing that its asymptotic behavior is consistent both with Poisson distributions and truncated power-laws. In order to study the large time behavior of the opinion dynamics we derive a mean-field description which allows to compute exact stationary solutions in some simplified situations. Structure preserving numerical methods are hence employed to describe correctly the large time behavior of the system, see [4,5].

References