RED ESPAÑOLA DE SUPERCOMPUTACIÓN

# 13th USERS CONFERENCE 2019. Zaragoza, 18-19 September

**POSTER SESSION**

#1 Numerical simulation of non-premixed swirling flames

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The major aim of the research is to improve the stabilization of flames of poor stoichiometries by means of a swirling flow. This provides saving of fuel as well as a reduction of contaminant emissions. Swirling burners have some advantages when compared with bluff bodies and cross flows. These are lower head losses and soot, less maintenance tasks. This work is devoted to gain an insight of flow pattern associated with different swirl numbers and diffusers. Axial swirl injector is composed by a certain number of fixed vanes in the annular nozzle. The Swirl number is associated with the angle of the trailing edge of the vanes. Besides, the influence of conical diffusers in the flame performance is analysed. To sum up, the strong swirl number had the lead stagnation point near the discharge of the nozzles and provided a reaction length lower than half diameter of the chamber. Intermediate swirl number have bigger Outer Recirculation Zones and the reaction length is more than one diameter. Finally the low swirl number do not have any vortex breakdown and the reaction length has several diameters. Bearing in mind the influence of conical diffusers, it is more important in the case of intermediate swirl numbers since the diffuser reduces the reaction length. These models were tested at a temporal resolution of 10-6 s/timestep, with spatial resolution 5 times larger than the Kolmogorov scale. It was found that for a mesh of 10 million cells without multigrid, the optimum is 360 processors. The authors acknowledge PRACE for awarding us access to the resource Curie-GENCI@CEA based in France and MareNostrum@BSC based in Spain. Ref. 2010PA1766. We acknowledge that the results of this research have been achieved using the DECI resource ARIS based in Greece at GRNET with support from the PRACE aisbl (ref. SWIRLLES Tier-1, DECI-14).

#2 Pressure induced effects of β-As2Te3

**E. Lora da Silva, R. I. Vilaplana, Instituto de Diseño para la Fabricación y Producción Automatizada, Universitat Politècnica de València**

The A2B3 compounds, with R-3m symmetry, have stimulated enormous research activity, because of their exceptional thermoelectric properties. More specifically, As2Te3 has shown some interesting properties and applications, which include memory devices, thermoelectric properties, conduction mechanism, and pressure-induced amorphisation to crystalline transition. β-As2Te3 is an isostructural form to layered Bi2Te3 and is known for displaying good thermoelectric properties. Moreover, the interest evidenced in such systems is the possibility of pressure-inducing electronic topological transitions (ETT) which can result in significant enhancements of their thermoelectric properties.

#3 Learning by doing on computational fluid dynamics

**Maria T. Parra, University of Valladolid**

**José M. Molina Jordá, University of Alicante**

This work involves the methodology used in the University of Valladolid for Mechanical Engineering students to learn Computational Fluid Dynamics playing an active role. Students carry out a fluid mechanics down scaled projects with the steps of sensibility of mesh, convergence of numerical algorithm, validation of turbulence model and description of flow patterns. Students pretend to be engineers in a consulting or design office carrying out a fluid mechanics scale down projects. Later they act as reviewers evaluating a project from a colleague. The offer of benchmark test cases ranges from head loses, driven cavities, swirling flows, to external aerodynamics. A review of the offer of workshops is supplied, such as the Ahmed car, the Roback and Johnson burner, aerodynamics of different NACA airfoils, and different geometries of driven cavities. These are classical test cases of numerical research and a sample of applications in wind energy, industrial furnaces, and lubrication. There is a deeper understanding of the topic when they need to discuss the strategies to accomplish the project, to write a technical report and finally to justify the evaluation of other works. Furthermore, they develop their critical thought, writing skills and synthesis capacity.

#4 Selective ethylene dimerization under intrapore condensation regime with defect-engineered Ru-HKUST-1 catalysts

**Manuel A. Ortuño, Institute of Chemical Research of Catalonia, Spain**

**Iker Agirrezabal-Telleria, University of the Basque Country, Spain**

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The production of 1-butene, a major monomer in polymer industry, is mostly dominated by ethylene dimerization processes. Although homogeneous catalysts are quite selective, they usually lack the robustness and recyclability of heterogeneous materials. In this scenario, metal–organic frameworks come into play to bridge the gap between these two worlds.

#5 Analysis of hybrid quantum-classical algorithms for optimization

**Pablo Diez-Valle, Consejo Superior de Investigaciones Científicas**

**Juan José García-Ripoll, Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas**

A promising paradigm for the resolution of optimization problems using quantum techniques is the known as hybrid quantum-classical algorithm. This kind of algorithms combines quantum computing via the variational method, and classical computing to optimize the variational parameters. In this work we focus on the resolution of Quadratic Unconstrained Binary Optimization problems (QUBO) since a broad spectrum of combinatorial optimization problems can be represented as a QUBO. The efficiency of the hybrid algorithms depends on several variables as the depth of the quantum circuit, the chosen ansatz, the classical method used to optimize the variational parameters, the entanglement etc. Our goal is to study how the mentioned conditions affect the performance in order to design more efficient optimization algorithms based on the variational method. We use the supercomputer Altamira Supercomputer at the Institute of Physics of Cantabria (IFCA-CSIC), member of the Spanish Supercomputing Network, to perform simulations which emulate a fully fault-tolerant quantum computer before running our algorithms on a real noisy quantum device. This research shall prepare for the Noisy Intermediate-Scale Quantum (NISQ) technology which will be available in the near future.

#6 Self-assembly of polymers interacting with the square well potential

**Miguel Herranz, Manuel Santiago, Nikos Karayiannis Manuel Laso, Departamento de Ingeniería Química y Medio Ambiente, ETSII, Universidad Politécnica de Madrid, UPM**

Self-assembly and crystallization of polymeric systems are closely related to processes and applications in engineering, biology, material, polymer and colloidal science. The aim of the present work is to study, through extensive simulations, how attractive interactions affect the ability of polymers to form clusters and eventually crystallize. We consider polymers as linear, freely-jointed chains of spheres of uniform size. The monomeric pair-wise interaction is a short-range potential of the "square well/shoulder" type. This model is defined by two parameters: σ_2, the range of interaction, and ε, the strength of the interaction. If ε is positive, it corresponds to repulsion (square shoulder); whereas negative values of ε lead to attraction between the monomers (square well). Simulations are carried out with a Monte Carlo scheme based on local and chain-connectivity-altering moves. Given the wealth of simulation results, we are able to con struct the phase diagram as a function of intensity and range of potential. If the strength of the attraction reaches a threshold value (ε<-0.6), polymeric chains self-assemble into clusters. Depending on the interaction strength these clusters may remain amorphous or transit to a stable, crystal phase. The higher the value of the interaction range, the more spherical and stable is be the cluster and the easier for the cluster to crystallize. We also study the bond gap effect and compare it against the strict tangency condition. Three different ordered morphologies are observed: random hexagonal close packing, sectors of mixed fcc/hcp character randomly meeting at twin axes occupied by sites of fivefold local symmetry and pure hcp/fcc crystals. Authors acknowledge support through project "MAT2015-70478" of MINECO. We thankfully acknowledge the computer resources and technical expertise and assistance provided by the Centro de Computacion y Visualizacion de Madrid (CeSViMa) through projects "p208" and "q373" and the Barcelona Supercomputing Center (BSC) through project "FI-2019-2-0014".

#7 DFT calculations approach for PbMoO4 and Pb1-2XCaXSrXMoO4 (x= 0.1, 0.2, 0.3, 0.4 and 0.5) solid solutions

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First-principles calculations were performed to provide a deep understanding of the local structures, bonding, morphologies, band gaps, and electronic and optical properties and open the door to exploit the electrical, optical and photocatalytic activity of this very promising family of materials. The geometries, electronic structures, and morphologies of as-synthetized of the PbMoO4 and Pb1-2XCaXSrXMoO4 (x= 0.1, 0.2, 0.3, 0.4 and 0.5) solid solutions samples were characterized by first-principles quantum-mechanical, based on the density functional theory [1]. By using Wulff construction and the values of the surface energies for the (001), (100), (110), (111), (011) and (112) crystal surfaces, a complete map of the available morphologies for PbMoO4 were obtained [2]. Good agreement between theoretical and experimental morphologies obtained from FE-SEM images is achieved [3].

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[2] Oliveira, Marisa. C. et al. 2016. “On the Morphology of BaMoO4 Crystals: A Theoretical and Experimental Approach.” Crystal Research and Technology 51(10): 634–44.
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#8 An atomistic understanding of the 2DEG at the LaAlO3-SrTiO3 interface

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Research involving new integration of semiconductor thin films is of interest, and has led to renewed research because such devices may exhibit innovative properties [1,2]. The two-dimensional electron gas (2DEG) at the interface of two otherwise insulating metal oxides, SrTiO3 (STO) and LaAlO3 (LAO), the LAO/STO heterostructure, has been investigated. The calculations were carried out by using density functional theory (DFT) as implemented in the Vienna Ab-initio simulation package (VASP) program [3]. The interfaces made by the co-exposed surfaces at LAO/STO were calculated by using an explicit atomistic model. The interaction between (LaO)+−(SrO)0, (LaO)+−(TiO2)0, (AlO2)−−(SrO)0, and (AlO2)−−(TiO2)0 layers in function of termination type, excess O anions on the upper part of the heterostructure, and interatomic distance at interface was evaluated. Interaction composed of the (AlO2)−−(TiO2)0 layers increase the interatomic distance, and when is formed by the (LaO)+−(SrO)0 interface exhibits a negative charge, implies that there is a repulsive force between them, and the electrons can be repelled. Excess of O-anions in the upper part of the heterostructure is able to eliminate the oxygen vacancies present; then, a complete local coordination, [AlO_6] and [LaO_12] cluster, are formed. The excess of O anions in the [TiO_5]-[AlO_5] model does not significantly affect the values of the Mulliken charge of these clusters, despite an increase occurring in the interatomic distance between the STO and LAO (100) surfaces. Our study introduces the possibility of defect engineering through the manipulation of oxygen vacancies and facet control at the interface and surface of materials, which can be ultimately be helpful in understanding the formation mechanisms of 2DEG at metal oxide interfaces.

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#9 HPC based study: Analysis on two systems: wild-type Kras4B and phosphorylation at S-181 of G12D bounded K-ras4B anchored into negatively charged cholesterol/DOPC/DOPS(15:28:7) plasma membrane

**Huixia Lu, Jordi Martí, Physics Department, UPC Barcelona Tech**

All Ras proteins family members belong to a class of protein called small GTpase. It plays an essential role in signal transduction pathways which ultimately turn on genes involved in cell growth, differentiation and survival so that overactive Ras signalling can lead to cancer. At normal levels, cholesterol is an essential substance for the body and it is present in every cell of the body and has important natural functions. Taking cholesterol into consideration could help us simulate more life-like cell membrane systems than those without cholesterol. Here in my study, I choose two systems: wild-type and oncogenic Kras4B anchored in a negatively charged membrane consists of cholesterol (30 mol%), DOPC (56 mol%) and DOPS (14 mol%), in which the ratio of DOPC:DOPS is 4:1. After running standard molecular simulation for both systems for 400 ns, short well-tempered metadynamics simulations were started for testing better

parameters of selected collective variables. Also standard molecular simulations were continued until 700 ns for collecting and averaging data. Interesting and novel results are presented in the conclusion part.

#10 PyCOMPSs - An Efficient Programming Framework for large scale data analytics for HPC

**Daniele Lezzi, Javier Alvarez, Pol Alvarez, Javier Conejero, Marc Domínguez, Jorge Ejarque, Hatem Elshazly, Francesc Lordan, Cristian Ramon-Cortes, Sergio Rodríguez, Salvi Solà, Rosa M. Badia, Barcelona Supercomputing Center**

This poster presents the latest updates on PyCOMPSs, a programming framework well suited for the scalable execution of scientific applications on distributed infrastructures including clouds and supercomputing clusters. In particular, we present the dislib library, a distributed machine learning library built on top of PyCOMPSs that addresses the issues of implementing and efficiently running machine learning algorithms on HPC resources. The dislib library not only eases the implementation phase, providing out of the shelf parallel implementations fo ML algorithms, but also demonstrates to scale the execution with large data sets overperforming other popular distributed machine learning libraries, such as MLlib.

#11 Toxicity prediction: HPC simulation meets machine learning

**Daniel Soler, Robert Soliva, Lucía Díaz, Suwipa Saen-Oon, Nostrum Bio Discovery, NBD**

The attrition rate of drug candidates amounts to up to 96% (Paul et al., 2010): Drug safety accounts for 30% of drug failures (Giri and Bader, 2015). Reliable methods to assess compound toxicity early on in drug discovery are thus needed. However, published studies on predicting small molecule toxicity are almost exclusively ligand-based. Most tools incorporate some means of molecular similarity, functional group propensities, molecular descriptors, QSAR or machine learning (ML). Therefore, we have concentrated our efforts on the High Risk-Off Target (HROT) set published by the Altman group at Stanford. These are 83 proteins that are predicted to bind low-dose drugs more frequently than high-dose drugs, i.e. proteins that are related to drugs which are administered at very low doses, because high doses lead to adverse events. Assessing whether small molecules interact with HROTs is useful in all phases of drug discovery. We are in the process of building a user-friendly plat form to discriminate in a high-throughput manner whether compounds are toxic (binding to HROTs) or not. The workflow consists in extracting 10 representative clusters from each molecular dynamics. Next, a curated dataset of active and decoy compounds are docked into these clusters. The docking scores are then used to train different machine learning models, so as to obtain a consistent and robust classifier that can predict whether a given compound hits an HROT target. We have so far tested this approach on three systems: The androgen receptor (394 actives/404 decoys), CYP3A4 (168 actives/168 decoys), and the beta-2 adrenergic receptor (230 actives/230 decoys) with successful results. In the near future, we plan to apply our methodology to a subset of the most important cytochromes and many more systems.