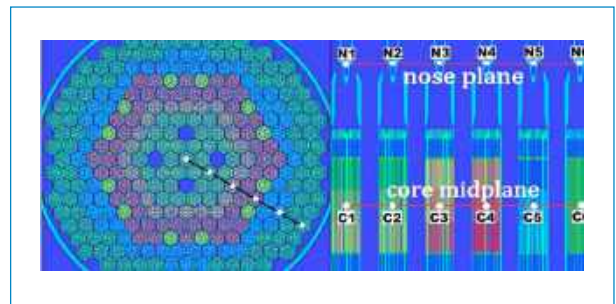
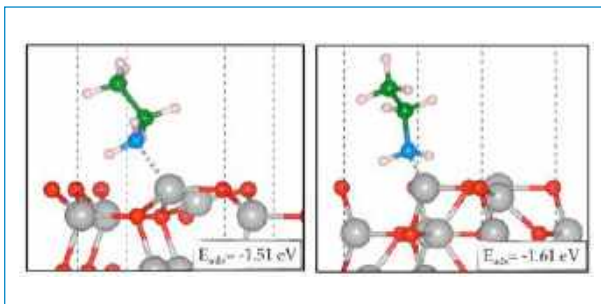
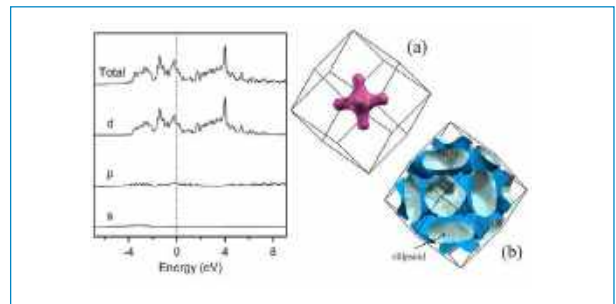
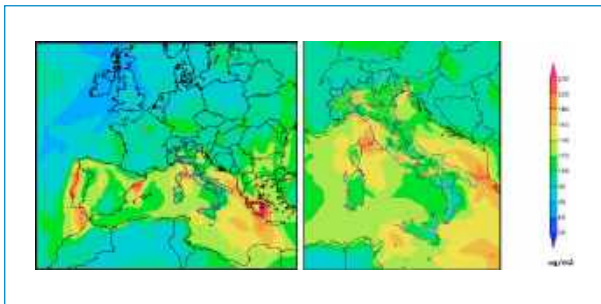
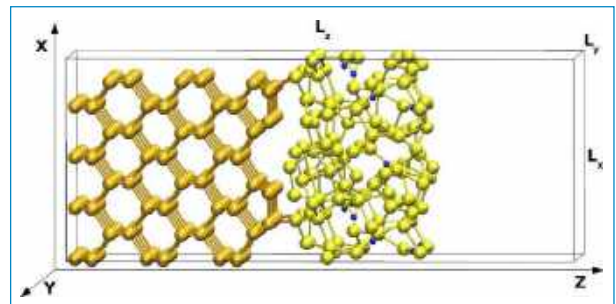
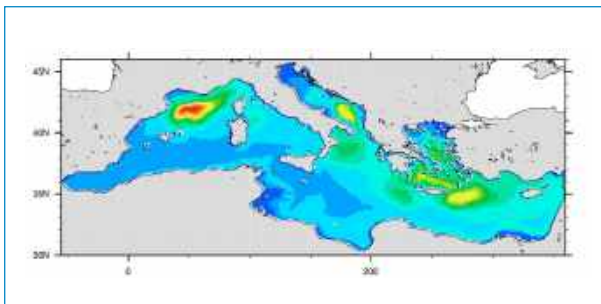


# High Performance Computing on CRESCO infrastructure: research activities and results 2015



**High Performance Computing on CRESCO Infrastructure:  
research activity and results 2015**

Contributions provided by a selection of users of the CRESCO infrastructure Scientific

Editor: *Giovanni Ponti*, ENEA, DTE-ICT-HPC, Research Centre Portici

Acknowledgements: We wish to thank *Gianclaudio Ferro* for providing the Reporter system (<http://hdl.handle.net/10840/5791>) to collect contributions and to build the Volume

Cover: *Amedeo Trolese*, ENEA, DTE-ICT-PRA, Research Centre Frascati

ISBN: 978-88-8286-342-5

## Contents

<i>Foreword</i>	5
<i>Ab Initio Carr-Parrinello Simulations of High Temperature GeO<sub>2</sub>: a comparison of the effects of plane waves cut-off and time step choice</i>	
<i>G. Mancini, M. Celino</i>	6
<i>Effects of preferential diffusion on turbulent lean premixed CH<sub>4</sub>/H<sub>2</sub> - Air slot flames</i>	
<i>D. Cecere, E. Giacomazzi, N.M. Arcidiacono, F.R. Picchia</i>	10
<i>A homemade Fortran code to analyse results from CPMD Calculations</i>	
<i>E. Burresti, M. Celino</i>	16
<i>Inter-layer synchronization in multiplex networks</i>	
<i>I. Sendiña-Nadal, I. Leyva, R. Sevilla-Escoboza, R. Gutiérrez, J.M. Buldú, J.A. Almendral, S. Boccaletti</i>	21
<i>Atmospheric Pollution Trends simulated at European Scale in the framework of the EURODELTA 3 Project</i>	
<i>G. Briganti, A. Cappelletti, M. Mircea, M. Adani, M. D'Isidoro</i>	26
<i>MCNP simulations supporting PWR GEN-II and III safety studies and feasibility study of minor actinides irradiation in the Tapiro research reactor</i>	
<i>P. Console Camprini, K. W. Burn</i>	31
<i>Monte Carlo study of dose-area-product properties in radiotherapy photon beams with small field sizes</i>	
<i>Claudio Caporali</i>	35
<i>Simulations of linear and nonlinear interactions between alfvén modes and energetic particles</i>	
<i>S. Briguglio, G. Fogaccia, V. Fusco, M. Martone, G. Vlad, X. Wang, T. Wang</i>	39
<i>Analysis of the wave field in front of the U-OWC</i>	
<i>P. Filianoti, L. Gurnari</i>	48
<i>A novel charge-equilibration method for self assembly of organics on metal surface</i>	
<i>A. Palma, M. Satta, S. Tosti</i>	52

<i>Enlightening of water self-assembling phenomena onto the (101) TiO<sub>2</sub> anatase surface by atomistic multi-scale modeling</i>	
<i>F. Gala, L. Agosta, G. Zollo</i>	56
<i>Implementation of an air quality forecast system over Italy</i>	
<i>M. Adani, M. D'Isidoro, G. Briganti, A. Cappelletti</i>	63
<i>First-principles investigation of the amino acids adsorption to hydrated non-polar ZnO surface</i>	
<i>F. Buonocore, C. Arcangeli, M. Celino, F. Gala, G. Zollo</i>	68
<i>Performance analysis of CRESCO clusters by using DGEMM subroutine</i>	
<i>Simone Giusepponi</i>	74
<i>CFD Simulations of hydrocarbons reforming with CO<sub>2</sub> capture in a fluidised bed carbonator</i>	
<i>A. Di Nardo, S. Stendardo, G. Calchetti</i>	80
<i>CP2K performance on CRESCO4 HPC system</i>	
<i>M. Gusso</i>	84
<i>Ab-initio study of silicon based materials for photovoltaic applications</i>	
<i>S. Giusepponi, M. Gusso, M. Celino, U. Aeberhard, P. Czaja</i>	88
<i>Quantum Espresso performance on ENEA and JSC HPC infrastructures</i>	
<i>S. Giusepponi, M. Gusso, M. Celino, U. Aeberhard, P. Czaja</i>	93
<i>Electronic band structure, lattice dynamics, and related superconducting properties of niobium from first-principles calculations</i>	
<i>G. De Marzi</i>	99
<i>Language discrimination via a neural network approach</i>	
<i>A. Mariano</i>	105
<i>Web Crawling tool integration in ENEAGRID</i>	
<i>G. Santomauro, G. Ponti, F. Ambrosino, G. Bracco, A. Colavincenzo, A. Funel, G. Guarnieri, S. Migliori, M. De Rosa, D. Giammattei</i>	110
<i>Fast switching alchemical simulations: a non equilibrium approach for drug discovery projects on parallel platforms</i>	
<i>P. Procacci</i>	115

<i>Simulation of photon beams for radiotherapy application</i>	
<i>L. Silvi, M. Pimpinella</i>	124
<i>Transport study of Neon impurity seeded FTU plasma by Gyrokinetic simulations</i>	
<i>V. Dolci, C. Mazzotta, FTU team</i>	129
<i>Self-Assembly of Triton X100 in Water Solutions: A Multiscale Simulation Study Linking Mesoscale to Atomistic Models</i>	
<i>A. De Nicola, Z. Ying, M. Celino, M. Rocco, T. Kawakatsu, G. Milano</i>	135
<i>Computer Simulation of Triglycerides</i>	
<i>A. Pizzirusso, Y. Zhao, A. De Nicola, G. Milano</i>	141
<i>Biconnectivity of Very Large Social Graphs</i>	
<i>G. Chiapparo, U. Ferraro Petrillo, D. Firmani, L. Laura</i>	144
<i>Do emission policies reduce ozone risk to European forests?</i>	
<i>A. Anav, A. De Marco</i>	148
<i>Multidecadal hindcast of the mediterranean thermohaline circulation</i>	
<i>G. Sannino, A. Carillo, M.V. Struglia</i>	151
<i>The core design of Gen-IV Lead Fast Reactors using the ERANOS code on the CRESCO HPC infrastructure</i>	
<i>M. Sarotto, G. Grasso, F. Lodi</i>	155
<i>Surface functionalization of ZnO for solar energy conversion devices: new insights from a first-principles study</i>	
<i>A.M. Rodríguez, A.B. Muñoz-García, C. De Rosa, M. Pavone</i>	159
<i>Car-Parrinello molecular dynamics of liquid NaNO<sub>3</sub></i>	
<i>R. Grena, M. Celino</i>	164
<i>First-principle determination of equilibrium and out of equilibrium excited state properties of surfaces and 2D materials</i>	
<i>M. Marsili, O. Pulci, M.S. Prete, A. Mosca Conte, P. Gori</i>	168
<i>Study of the Zr Doping in the Cerium Oxide through First-Principles Calculations</i>	
<i>F. Rizzo, G. De Marzi</i>	174
<i>The influence of TiO<sub>2</sub> and Ti dopants on the hydrogen mobility through MgH<sub>2</sub>-Mg interface</i>	
<i>R. Vujasin, J. Grbovic Novakovic, N. Novakovic, S. Giusepponi, M. Celino</i>	178

<i>The phase structure of the Naming Game in the stochastic block model</i>	
<i>F. Palombi, S. Toti</i>	182
<i>Transcriptome assembly of C. sativus</i>	
<i>A. Conte, G. Aprea, M. Pietrella</i>	187
<i>Analysis of current fast neutron-flux monitoring instrumentation targeted for the DEMO LFR ALFRED</i>	
<i>L. Lepore, R. Remetti, M. Cappelli</i>	192
<i>Analysis of the chaotic behavior of the Lower Hybrid Wave propagation in magnetised plasma by Hamiltonian theory</i>	
<i>A. Cardinali, A. Casolari</i>	198
<i>Bi(111) nanofilms: quantum confinement and surface states</i>	
<i>G. Cantele, D. Ninno</i>	202
<i>Multiphase rotating turbulent flows in gas turbine internal cooling channel</i>	
<i>D. Borello, F. Rispoli, A. Salvagni, P. Venturini</i>	206
<i>CRESCO numerical combustion analysis of swirling micro-meso combustion chambers</i>	
<i>A. Minotti</i>	210
<i>CFD modeling of a flameless furnace: comparative evaluation of turbulent combustion models with two software on a HPC platforms</i>	
<i>C. Mongiello, G. Guarneri, G. Continillo, D. Iorio, G. Maio, F.S. Marra</i>	214
<i>Role of the sub-surface vacancy in the amino-acids adsorption on the (101) anatase TiO<sub>2</sub> surface: a first principles study</i>	
<i>L. Maggi, F. Gala, G. Zollo</i>	220
<i>Neutronics calculations for the design of DEMO WCLL reactor</i>	
<i>R. Villari, G. Mariano, A. Del Nevo, D. Flammini, F. Moro</i>	227
<i>The network architecture underlying the CRESCO infrastructure of ENEA Portici</i>	
<i>D. Giammattei, M. De Rosa, A. Colavincenzo, R. Guadagni</i>	231