

## CONTENTS

Workshop photographs	v
Organizing Committees	vi
Preface	vii
Memory of Livio Scarsi	ix
<b>Part A — Astrophysics, Cosmology and Earth Physics</b>	<b>1</b>
Simulations for UHE Cosmic Ray Experiments <i>J. Knapp</i>	3
Detector Modeling in Astroparticle Physics <i>S. Petrerá</i>	12
Simulating a Large Cosmic Ray Experiment: The Pierre Auger Observatory <i>T. Paul</i>	23
Testing of Cosmic Ray Interaction Models at LHC Collider <i>P. Nečesal, J. Řídký</i>	32
Observations, Simulations, and Modeling of Space Plasma Waves: A Perspective on Space Weather <i>V. S. Sonwalkar</i>	39
Electron Flux Maps of Solar Flares: A Regularization Approach to Rhessi Imaging Spectroscopy <i>A. M. Massone, M. Piana, M. Prato, A. G. Emslie, G. J. Hurford, E. P. Kontar, R. A. Scwartz</i>	48
Problems and Solutions in Climate Modeling <i>A. Sutera</i>	55

Numerical Simulations and Diagnostics in Astrophysics: A few Magnetohydrodynamics Examples	66
<i>G. Peres, R. Bonito, S. Orlando, F. Reale</i>	
Numerical Simulations of Multi-Scale Astrophysical Problems: The example of Type Ia Supernovae	74
<i>F. K. Röpke</i>	
Numerical Simulations in Astrophysics: From the Stellar Jets to the White Dwarfs	83
<i>F. Rubini, L. Delzanna, J. A. Biello, J. W. Truran</i>	
Statistical Analysis of Quasar Data and Validity of the Hubble Law	90
<i>S. Roy, J. Ghosh, M. Roy, M. Kafatos</i>	
Non-Parametric Tests for Quasar Data and Hubble Diagram	99
<i>S. Roy, D. Datta, J. Ghosh, M. Roy, M. Kafatos</i>	
Doping: A New Non-Parametric Deprojection Scheme	107
<i>D. Chakrabarty, L. Ferrarese</i>	
Quantum Astronomy and Information	114
<i>C. Barbieri</i>	
Mining the Structure of the Nearby Universe	125
<i>R. D'Abrusco, G. Longo, M. Brescia, E. De Filippis, M. Paolillo, A. Staiano, R. Tagliaferri</i>	
Numerical Characterization of the Observed Point Spread Function of the VST Wide-Field Telescope	134
<i>G. Sedmak, S. Carrozza, G. Marra</i>	
<b>Part B — Biology, Biochemistry and Bioinformatics</b>	<b>141</b>
From Genomes to Protein Models and Back	143
<i>A. Tramontano, A. Giorgetti, M. Orsini, D. Raimondo</i>	
Exploring Biomolecular Recognition by Modeling and Simulation	150
<i>R. Wade</i>	

From Allergen Back to Antigen: A Rational Approach to New Forms of Immunotherapy	154
<i>P. Colombo, A. Trapani, D. Geraci, M. Golino, F. Gianguzza, A. Bonura</i>	
Sulfonylureas and Glinidies as New PPAR $\gamma$ Agonists: Virtual Screening and Biological Assays	158
<i>M. Scarsi, M. Podvinec, A. Roth, H. Hug, S. Kersten, H. Albrecht, T. Schwede, U. A. Meyer, C. Rücker</i>	
A Multi-Layer Model to Study Genome-Scale Positions of Nucleosomes	169
<i>V. Di Gesù, G. Lo Bosco, L. Pinello, D. Corona, M. Collesano, G.-C. Yuan</i>	
BioInfogrid: BioInformatics Simulation and Modeling Based on Grid	178
<i>L. Milanesi</i>	
Geometrical and Topological Modelling of Supercoiling in Supramolecular Structures	187
<i>L. Boi</i>	
<b>Part C — Methods and Techniques</b>	<b>201</b>
Optimisation Strategies for Modelling and Simulation	203
<i>J. Louchet</i>	
Modeling Complexity using Hierarchical Multi-Agent Systems	213
<i>J.-C. Heudin</i>	
Topological Approaches to Search and Matching in Massive Data Sets	224
<i>F. Murtagh</i>	
Data Mining: Computational Theory of Perceptions and Rough-Fuzzy Granular Computing	234
<i>S. K. Pal</i>	
Biclustering Bioinformatics Data Sets: A Possibilistic Approach	246
<i>F. Masulli</i>	
Supervised Automatic Learning Models: A New Perspective	255
<i>E. F. Sánchez-Úbeda</i>	

Interactive Machine Learning Tools for Data Analysis	264
<i>R. Tagliaferri, F. Iorio, F. Napolitano, G. Raiconi, G. Miele</i>	
Data Visualization and Clustering: An Application to Gene Expression Data	272
<i>A. Ciaramella, F. Iorio, F. Napolitano, G. Raiconi, R. Tagliaferri, G. Miele, A. Staiano</i>	
Super-Resolution of Multispectral Images	279
<i>R. Molina, J. Mateos, M. Vega, A. K. Katsaggelos</i>	
From the Qubit to the Quantum Search Algorithms	287
<i>G. Cariolaro, T. Occhipinti</i>	
Visualization and Data Mining in the Virtual Observatory Framework	295
<i>M. Comparato, U. Becciani, B. Larsson, A. Costa, C. Gheller</i>	
An Archive of Cosmological Simulations and the ITVO Multi-Level Database	300
<i>P. Manzato, R. Smareglia, L. Marseglia, V. Manna, G. Taffoni, F. Gasparo, F. Pasian, C. Gheller, V. Becciani</i>	
Studying Complex Stellar Dynamics using a Hierarchical Multi-Agent Model	307
<i>J.-C. Torrel, C. Lattaud, J.-C. Heudin</i>	
AIDA: Astronomical Image Decomposition and Analysis	313
<i>M. Uslenghi, R. Falomo</i>	
Comparison of Stereo Vision Techniques for Cloud-Top Height Retrieval	319
<i>A. Anzalone, F. Isgró, D. Tegolo</i>	
Author Index	327
Participants	329