CEBA'13	PROGRAMME		
Monday	1-Jul-13		
9:00		**REGISTRATION**	
9:15	Walter Rocchia	Welcome and introduction	
	Dept. of Drug Discovery and Development, IIT (ITA)		
	SESSION 1	**ELECTROSTATICS IN BIOLOGICAL SYSTEMS**	
9:30	Benoit Roux	Electrostatics in biomolecular systems	Opening Keynote Lecture
	Biochemistry and Molecular Biophysics, University of Chicago (USA)		
10:30	Jim Warwicker	Electrostatics models for Biology	
	University of Manchester (UK)		
11:00		Coffee Break	
	SESSION 2	**SOLVENT MODELS**	
11:30	Jan Forsman	Classical density functional theories of ionic solutions	invited lecture
	Lund University (SE)		
12:30	Alexey Onufriev	Introducing charge hydration asymmetry into continuum electrostatics framework	
	Virginia Tech (USA)		
13:00		Lunch	
	SESSION 3	**NUMERICAL APPROACHES AND SOLVERS**	
14:00	Walter Rocchia	Continuum electrostatics for Biological Applications: the DelPhi case	
	Dept. of Drug Discovery and Development, IIT (ITA)		
14:30	Paola Pietra	Discontinuous Galerkin schemes for elliptic problems	invited lecture
	IMATI – CNR (ITA)		
15:00	Alexander Boschitsch	Surface Electrostatics Using An Adaptive Cartesian Grid-Based Poisson-Boltzmann Solver	invited lecture
	Continuum Dynamics, Inc., Ewing, New Jersey (USA)		
15:30	Frederic Gibou	An Adaptive, Finite Difference Solver for the Non- linear Poisson-Boltzmann Equation with Applications to Biomolecular Computations	
	University of California Santa Barbara (USA)		
16:00		Coffee Break	
16:30	Donald Bashford	Design, Development and Applications of the MEAD Suite for Macromolecular Electrostatics	invited lecture
	Saint Jude Children's Research Hospital (USA)		
17:00	Jaydeep P. Bardhan	Progress and Challenges in Boundary-Integral Methods for Biological Electrostatics	invited lecture
	Dept. Electrical and Computer Engineering, MIT (USA)		
18:00	Sergei Grudinin	Efficient Boundary Element Method with curved elements for implicit solvation in biological systems	
	INRIA/CNRS (FR)		
18:30	Federico Fogolari	Generalized Born forces: surface integral formulation.	
	University of Udine (ITA)		

Tuesday	2-Jul-13		
9:00	Michela Spagnuolo	Introduction	
	IMATI – CNR (ITA)		
	SESSION 4	**MOLECULAR SURFACE MODELS**	
9:15	Nico Kruithof	Molecular surface design with balls	invited lecture
	SURFsara (NL)		
10:00	Giuseppe Patané	State-of-the-art and perspectives of implicit modeling for molecular surfaces	invited lecture
	IMATI – CNR (ITA)		
10:45	Coffee Break		
11:15	Alexander Boschitsch	The Role of Molecular Surface Definition in the Emergence of Singular Solutions to the Poisson-Boltzmann Equation	invited lecture
	Continuum Dynamics, Inc., Ewing, New Jersey (USA)		
12:00	Pierre Alliez	A Generic Framework for Delaunay Mesh Generation and Optimization	invited lecture
	INRIA Sophia-Antipolis – Mediterranée (FR)		
13:00		Lunch	
	SESSION 5	**BROADENING THE VIEW**	
14:00	Guowei Wei	Multiscale multiphysics and multidomain models for biomolecular systems	Keynote Lecture
	Michigan State University (USA)		
15:00	Monica Zoppe'	Beyond computation, the representation of electrostatics in biological settings	
	Scientific Visualization Unit IFC - CNR (ITA)		
15:30	Coffee Break		
	SESSION 6	**DEALING WITH COMPUTATIONAL COMPLEXITY**	
16:00	Sergio Decherchi	NanoShaper: a general and robust ray-casting based tool for processing surfaces at the nanoscale	
	Dept. of Drug Discovery and Development, IIT (ITA)		
16:30	Sérgio E. Dias	Triangulating Molecular Surfaces with Millions of Atoms	
	Dept. of Computing, University of Beira Interior (PT)		
17:00	José Colmenares	Mixed MPI-CUDA implementation of full PB equation	
	Dept. of Drug Discovery and Development, IIT (ITA)		
19:45	**SOCIAL EVENT: POSTER SESSION AND GUIDED TOUR OF THE GENOA ACQUARIUM**		

Wednesday	3-Jul-13		
	SESSION 7	**APPLICATIONS TO BIOLOGY AND BIOPHYSICS**	
9:30	Rosa Di Felice	Control of DNA Minor Groove Width and Electrostatic Potential in Fis Binding Sequences	
	CNR-NANO S3 Center (ITA)		
10:00	Michael Martinez	Computing protein binding properties from molecular electrostatic potentials	
	Heidelberg Institute for Theoretical Studies (DE)		
10:30	Jesper Sørensen	Comparative Poisson-Boltzmann equation calculations for binding free energies focusing on physical and algorithmic parameters	
	University of California San Diego (USA)		
11:00	Coffee Break		
11:30	Marcia Fenley	Biophysical Applications of the Adaptive Cartesian Grid Poisson-Boltzmann Equation Software Package	invited lecture
	Institute of Molecular Biophysics, Florida State University (USA)		
12:00	Mickey Kosloff	Structural and electrostatic determinants of interaction specificity in G-protein mediated signaling	invited lecture
	Department of Human Biology, University of Haifa (IL)		
12:30	Vittorio Limongelli	Free Energy Landscapes in Biological Systems	
	University of Naples "Federico II" (ITA)		
13:00		Lunch	
14:00	Goran Neshich	Using structural and physical-chemical parameters to identify functional districts in proteins - the role of electrostatic potential	invited lecture
	Computational Biology Research Group, EMBRAPA (BRA)		
	SESSION 8	**APPLICATIONS TO MATERIALS SCIENCE**	
14:30	Alain Delgado	Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle	
	CNR-NANO S3 Center (ITA)		
15:00	Vladimir A. Baulin	Modelling of spherical interpolyelectrolyte complexes	
	Universitat Rovira i Virgili (ES)		
15:30	**Conclusive Remarks**		
16:00	Coffee Break		
16:30:00 PM-18:00:00 PM	**"Hands on DelPhi" session**		