2nd BSC International Doctoral Symposium

5th, 6th & 7th May, 2015

2nd International BSC Doctoral Symposium 2015 – 5th May			
Start time	Activity	Speaker/s	Chair
9.00h	Welcome and opening	Mateo Valero, BSC Director	Maria Ribera, Education & Training Group Manager at BSC
9.15h	Keynote Speaker talk: Research in Telefónica R&D	Nuria Oliver, Scientific Director Telefónica R&D	
10.10h	First Poster Session & coffee break *Heating Bulk Ions in DEMO with ICRF waves* Dani Gallart, BSC Computer Applications in Science & Engineering Dpt. *Rayleigh wave ellipticity measurements in the Iberian Peninsula and Morocco* Clara Gómez-García, Spanish National Research Council *Implementation of Dynamic Aerosol-Radiation Interaction within the NMMB/BSC-CTM* Vincenzo Obiso, Earth Sciences Dpt. *State-of-the-Art Climate Predictions for Energy Climate Services* Verónica Torralba, Institut Català de Ciènces del Clima *Identification of novel type 2 diabetes susceptibility loci through wholegenome imputation using sequencing based reference panels into 13.201 cases and 59.656 controls* *Sílvia Bonàs Guarch, BSCLife SciencesDpt.* *Parallel programming issues and what the compiler can do to help* Sara Royuela, BSC Computer Sciences Dpt.		
First Talk Session: PostDoc research at BSC (first part)			
10.40h	Methodology to predict scalability of parallel applications	Claudia Rosas, BSC Computer Sciences Dpt.	Mariano Vázquez, High Performance Computational Mechanics Group Manager at BSC
11:00h	Mesh generation to simulate incompressible Navier-Stokes equations with wind turbines	Abel Gargallo-Peiró, BSC Computer Applications in Science & Engineering Dept.	
11.20h	Measurements and computer simulations: whom do we trust for atmospheric composition?	Enza Di Tomaso, BSC Earth Sciences Dept.	
11.40h	HPC and edge elements for geophysical electromagnetic problems: an overview	Octavio Castillo, BSC Computer Applications in Science & Engineering Dept.	
12.00h	Second Poster Session & coffee break *Automatic Query Driven Data Modelling in Cassandra* Roger Hernandez, BSC Computer Sciences Dept. *Modelling the Contact Propagation of Nosocomial Infection in Emergency Departments* Cecili Jaramillo, Universidad Autónoma de Barcelona *MACC: Mercurium ACCelerator Model* Guray Ozen, BSC Computer Sciences Dept. *Capturing the action of current antipsychotic drugs at G protein-coupled receptors (GPCRs) by means of Markov State Model analysis* Ismael Rodríguez-Espigares, Universitat Pompeu Fabra (UPF) - Hospital del Mar Medical Research Institute (IMIM) *A 3D-1D cardiac-vascular computational feedbacked model* Alfonso Santiago, BSC Computer Applications in Science & Engineering Dept.		

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Start time	Activity	Speaker/s	Chair
First Talk Session: PostDoc research at BSC (second part)			
12.20h	From imaging to simulation: a framework applied to simulate the blood flowin the carotids	Ruth Arís, BSC Computer Applications in Science & Engineering Dept.	José María Cela, Director of BSC Computer Applications in Science & Engineering Dept.
12:40h	Optimizing a coarse-grained model for the recognition of protein-protein binding	Agustí Emperador, BSC Life Sciences Dpt.	
13.00h	Lunch break		
15.00h	Training An Introduction to Scientific Writing starts; Lecturer Josep Lluis Pelegrí, ICM-CSIC		
17.00h	Coffee break		
17.15h	Training An Introduction to Scientific Writing continues; Lecturer Josep Lluis Pelegrí, ICM-CSIC		
19.00h	Adjourn		

2nd International BSC Doctoral Symposium 2015 – 6th May			
Start time	Activity	Speaker/s	Chair
9.00h	Opening of the second day		
Second Talk Session: Algorithms, Physics & Data Science			
9.10h	Study of Preconditioners based on Markov Chain Monte Carlo Methods	Oscar A. Esquivel (PostDoc), CONACYT-BSC Computer Sciences Dept.	Vassil Alexandrov , Extreme Computing Group Manager at BSC
9.30h	Supercomputing simulations for Beyond Standard Model theories at the TeV scale: non-standard gravity and electroweak interactions	Rafael Delgado, Universidad Complutense de Madrid	
9.50h	Discovering most significant news using Network Science approach	Ilya Blokh, Perm State University	
10.10h	Linompss – A Linear Algebra Library on OMPSs	Sicong Zhuang, BSC Computer Sciences Dept.	
10.30h	Third Poster Session & coffee break Evaluation of Modelling Systems in High Resolution to Assess the Air Pollutant Impacts on Human Health Sergio N. González (PostDoc), BSC Earth Sciences Dpt - CONACYT. *Binding Free Energy and Ligand Orientation Calculations using A Monte Carlo Method with Markov Sate Analysis* Daniel Lecina, BSCLife SciencesDept. *Asynchronous parallel fluid solver and particle transport* Edgar Olivares, BSC Computer Applications in Science & Engineering Dept. *A parallel coupled algorithm for the solution of deformable two-body contact problem* Matías Rivero, BSC Computer Applications in Science & Engineering Dept. *Resource Management for Software Defined Data Centers for Heterogeneous Infrastructures* Marcelo Amaral, BSC Computer Sciences Dept. *A framework for multidimensional indexes on distributed and highly-available data stores* Cesare Cugnasco, BSC Computer Sciences Dept. *Mathematical Representation of the Hardware Round-Robin Scheduler Analytical Model for Single-ISA Heterogeneous Architectures* Daniel Nemirovsky, BSC Computer Sciences Dept.		
Third Talk Session: Scheduling, Interconnections and Simulations			
11.20h	Criticality-Aware Dynamic Task Scheduling for Heterogeneous Systems	Kallia Chronaki, BSC Computer Sciences Dept.	Daniele Lezzi, Senior researcher at BSC Grid Computing and Clusters Group
11.40h	Interconnect Energy Savings on MapReduce Clusters	Renan Fischer e Silva, BSC Computer Sciences Dept.	
12.00h	Efficient Address Translation for Memory Intensive Workloads	Vasileios Karakostas, BSC Computer Sciences Dept.	
12.20h	High Performance Computing Based Simulation for Healthcare Decision Support	Zhengchun Liu, Universitat Autònoma de Barcelona	
12.40h	Hardware Scheduling Algorithms for Asymmetric Single-ISA CMPs	Nikola Markovic, BSC Computer Sciences Dept.	
13.00h	Lunch break		
15.00h	Training An Introduction to Scientific Writing continues; Lecturer Josep Lluis Pelegrí, ICM-CSIC		
17.00h	Coffee break		
17.15h	Training An Introduction to Scientific Writing continues; Lecturer Josep Lluis Pelegrí, ICM-CSIC		
19.00h	End of the Training and Adjourn		

2nd International BSC Doctoral Symposium 2015 – 7th May			
Start time	Activity	Speaker/s	Chair
9.00h	Opening of the third day		
Fourth Talk Session: Life Sciences			
9.10h	Macroscopic structures generated by microorganisms swimming in a fluid	Francisco Alarcón, Universitat de Barcelona	David Torrents, Computational Genomics Group Manager
9.30h	Assessment of scoring functions performance to re-rank docking decoys from FFT(Fast Fourier Transform) programs	Didier Barradas, BSC Life Sciences Dept.	
9.50h	Implementation of an Internal Coordinates Anisotropic Network Model in PELE	Víctor A. Gil, BSC Life Sciences Dept.	
10.10h	Inter-residue interactions in membrane proteins	Eduardo Mayol, Universitat Autònoma de Barcelona	
10.30h	Fourth Poster Session & coffee break *Galaxy Gears: Web Services integration into Galaxy workflows* Dmitry Repchevsky, BSCLife SciencesDept. *Single amino acid mutation controls hole transfer dynamics in DNAmethyltransferase HhaI complexes* Marina Corbella, Universitat de Barcelona *Catalytic surface radical in dye-decolorizing peroxidase* Marina Cañellas, BSCLife SciencesDept. *Theoretical study on the activation mechanism of AMP-kinase by means of Molecular Dynamics Simulations* Carolina Estarellas (PostDoc), Universitat de Barcelona *GWImp-COMPSs: An Integrated Framework for Large-scale Genome-wide Imputation and Association Testing* Marta Guindo, BSCLife SciencesDept. *PMut2015: a web-based tool for predicting pathological mutations on proteins* Víctor López, BSCLife SciencesDept. *Influence of Temperature on the Topological Features of Inner Cavities in Cytoglobin* Constantí Seira, Universitat de Barcelona *Cation- π-cation interactions in proteins* Silvana De Souza Pinheiro, Universitat de Barcelona		
Fifth Talk Session: Computer Sciences and Applications			
11.20h	A novel approach to reconstruct the plinian and co-ignimbrite phases of large eruptions - Campanian Ignimbrite	Alejandro Martí, BSC Computer Applications in Science & Engineering Dept.	Eduard Ayguadé, Associate Director of BSC Computer Sciences Dept.
11.40h	Plasma Physics Code Contribution to the Mont-Blanc Project	Xavier Sáez, BSC Computer Applications in Science & Engineering Dept.	
12.00h	Folding: reporting instantaneous performance metrics and source-code references	Harald Servat, BSC Computer Sciences Dept.	
12.20h	Probabilistically Time-Analyzable Complex Processors in Hard Real-Time systems	Mladen Slijepcevic, BSC Computer Sciences Dept.	
12.40h	Improving the prefetching performance through code region profiling	Martí Torrents, UPC BarcelonaTech	
13.00h	Lunch break		

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Sixth Talk Session: Earth Sciences and Physics			
14.00h	Dynamics of double-polarity subduction: application to the Western Mediterranean	Mireia Peral, Institute of Earth Science Jaume Almera (CSIC)	Arnau Folch, Environmental Simulations Group Manager at BSC
14.20h	Characterization of coal power plants plume dynamics under typical synoptic conditions over the Iberian Peninsula	Víctor Valverde, BSC Earth Sciences Dept.	
14.40h	Quantum dynamics study of the hydrogen molecule confined in single-walled carbon nanotubes	Manel Mondelo-Martell, Universitat de Barcelona	
15.00h	Fifth Poster Session & coffee break *Hecuba: NoSql made easy* Guillem Alomar, BSC Computer Sciences Dept. *Scaling Irregular Array-type Reductions in OmpSs* Jan Ciesko, BSC Computer Sciences Dept. *DLP Acceleration on General Purpose Cores* *Milovan Duric*, BSC Computer Sciences Dept. *Enhancing Timing Analysis for COTS multicores for the Space industry: a software approach* *Gabriel Fernandez, UPC BarcelonaTech* *Methodology to select a I/O configuration (hardware resources and stack software) in cloud platform* *Pilar Gómez, Universitat Autònoma de Barcelona* *A Multiphysics implementation for conjugate heat transfer and compressible-low mach coupling* *Miguel Zavala*, BSC Computer Applications in Science & Engineering Dept. *Undestanding Scientific Application's Performance* *Oriol Tintó , Universitat Autònoma de Barcelona*		
Seventh Talk Session: Life Sciences			
15.30h	Sugar Conformations that Enhance Cleavage of Glycosidic Bonds in Carbohydrate-Active Enzymes	Lluis Raich, Universitat de Barcelona	Víctor Guallar, Electronic and Atomic Protein Modelling Group Manager at BSC
15.50h	pyDock performance in 5th CAPRI edition: from docking and scoring to binding affinity predictions and other challenges	Chiara Pallara, BSC Life Sciences Dept.	
16.10h	Characterization of complex chromosomal rearrangements in cancer genomes	Marta Munar, BSC Life Sciences Dept.	
16.30h	Conclusions		
17.00h	End of the Doctoral Symposium		