

TOWARDS IN SILICO HUMANS: A CHALLENGE FOR EXASCALE COMPUTING AREA

PROGRAM

COSMOCAIXA. C/ ISAAC NEWTON, 26. BARCELONA

Wednesday, September, 18th, 2013**9:15 Welcome**

THE FUTURE OF SUPERCOMPUTING FOR LIFE SCIENCES

9:30 EU Strategy on HPC and its Implementation**Aniyan Varghese**, DG-CONNECT, European Commission, Brussels, Belgium**10:00 SESSION 1: EUROPEAN RESOURCES AND FUTURE SUPERCOMPUTING**Chair: **Alison Kennedy**, EPCC University of Edinburgh, UK**A Competence Centre for Life Science Applications****Erwin Laure**, KTH Royal Institute of Technology, Stockholm, Sweden**Reaching Exascale Through Many Simulations: Abstractions and Tools****Matteo Turilli**, Rutgers, New Jersey, USA**The Scientific Case for HPC in Europe 2012-2020. Perspectives from the Life Sciences****Martyn Guest**, University of Cardiff, Cardiff, United Kingdom**11:30 Coffee break****12:00 SESSION 2: INVESTING IN DISRUPTIVE TECHNOLOGY**Chair: **Francesc Subirada**, Barcelona Supercomputing Center, Barcelona, Spain**Creating Value in Life Sciences****Montserrat Vendrell**, Biocat, Barcelona, Spain**Frontier Research. The Role of Private Foundations****Pepa Limeres**, Fundación Botín, Madrid, Spain**Nanonica: a Business Angels Investment Company in Breakthrough Technologies****Aurora Conill**, Nanotargeting, Barcelona, Spain**Biotech Innovation & Development Models in an Evolving Market****Christian Suojanen**, Valor Management, Canada

B-DEBATE IS AN INITIATIVE OF:

WITH THE COLLABORATION OF:



TOWARDS IN SILICO HUMANS: A CHALLENGE FOR EXASCALE COMPUTING AREA

Wednesday, September, 18th, 2013

13:30 Lunch

15:00 SESSION 3: EUROPEAN EXASCALE SOFTWARE INITIATIVE

European Exascale Software Initiative: Evolution in Life Sciences Domain and Recommendations

Chair: **Charles Laughton**, University of Nottingham, Nottingham, United Kingdom

EESI Life Sciences Expert Panel

16:30 Coffee break

17:30 End of the session

Thursday, September, 19th, 2013

MULTI-SCALE SIMULATION OF LIVING ORGANISMS

9:30 SESSION 4: MOLECULAR SIMULATION

Chair: **Richard Lavery**, University of Lyon, Lyon, France

Multiscale Simulations of Membrane and Membrane Proteins

Paolo Carloni, German Research School, Aachen, Germany

Exascale Biomolecular Simulation. A Revolution or Evolution?

Erik Lindhal, KTH Royal Institute of Technology, Stockholm, Sweden

In-silico Molecular Recognition by Molecular Simulations

Gianni de Fabritiis, Universitat Pompeu Fabra, Barcelona, Spain

11:00 Coffee Break

B-DEBATE IS AN INITIATIVE OF:



WITH THE COLLABORATION OF:



TOWARDS IN SILICO HUMANS: A CHALLENGE FOR EXASCALE COMPUTING AREA

Thursday, September, 19th, 2013

11:30 SESSION 5: LIFE SYSTEMS SIMULATION

Chair: **Alfonso Valencia**, Centro Nacional de Investigaciones Oncológicas (CNIO), Madrid, Spain

Computational Biomedicine: Towards the Virtual Human
Peter Coveney, University College London, London, United Kingdom

TBD

Henry Markram, École Polytechnique Fédérale de Lausanne, Laussane, Switzerland

Alya Red CCM: Supercomputers in Cardiac Simulation
José María Cela, Barcelona Supercomputing Center, Barcelona, Spain

13:00 Lunch

SESSION 6: OPEN SYMPOSIUM

MULTI-SCALE SIMULATION OF LIVING ORGANISMS: FROM GENOMES TO ENTIRE HUMAN ORGANS

15:00 **Title to be defined.**
Henry Markram, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

15:40 **Mapping Origin and Impact of Structural Variants in Cancer**
Jan Korbel, European Molecular Biology Laboratory, Heidelberg, Germany

16:20 Coffee break

16:40 **Biology, as Part of the "Big Data Science" Movement**
Alfonso Valencia, Centro Nacional de Investigaciones Oncológicas (CNIO), Madrid, Spain

17:20 **The Role of Simulation in Clinical Decision Making**
Peter Coveney, University College London, London, United Kingdom

18:00 **Open debate**
Chair: **Modesto Orozco**, Barcelona Supercomputing Center, Barcelona, Spain

B-DEBATE IS AN INITIATIVE OF:



WITH THE COLLABORATION OF:

TOWARDS IN SILICO HUMANS: A CHALLENGE FOR EXASCALE COMPUTING AREA

Friday, September, 20th, 2013

FUTUR COMPUTING FOR PHARMACEUTICAL INDUSTRY

9:30 SESSION 7: COMPUTING FOR GENOMICS

Chair: **David Torrents**, Barcelona Supercomputing Center, Barcelona, Spain

The Genomics Interpretation Bottleneck, from the Personalized Genome to the Single-cell: the Challenges of Tertiary Analysis and Visualization

Eduardo González Couto, Integromics, Granada, Spain

Mapping Origin and Impact of Structural Variants in Cancer

Jan Korbel, European Molecular Biology Laboratory, Heidelberg, Germany

10:30 Coffee break

11:00 SESSION 8: COMPUTING FOR SYSTEMS BIOLOGY

Chair: **Patrick Aloy**, Institut de Recerca Biomèdica de Barcelona, Barcelona, Spain

Towards In-silico Organogenesis

James Sharpe, Center for Genomic Regulation (CRG), Barcelona, Spain

Systems Medicine: The Growing Discrepancy Between Available Data and Expectations from Simulations

Rob Russell, University of Heidelberg, Heidelberg, Germany

12:00 SESSION 9: COMPUTING FOR DRUG DISCOVERY

Chair: **Xavier Barril**, Universitat de Barcelona, Barcelona, Spain

Challenges and Opportunities for Computational Science in Drug Discovery

Darren Green, Glaxo Smith Kline, Stevenage, United Kingdom

Progressing Computational Advanced Physics-based and Knowledge-based Approaches in Drug Discovery

Edgar Jacoby, Janssen Research & Development, Beerse, Belgium

Molecular Simulation in Drug Discovery

Mike King, UCB, Slough, United Kingdom

13:30 Conclusions and closing remarks

B-DEBATE IS AN INITIATIVE OF:

WITH THE COLLABORATION OF:

