Full Programme

Wednesday 25th September

09:30 - 09:45	Welcome Address
Location: Kelvin Lecture Theatre Peter V. Coveney	

09:45 - 10:30	Keynote Address
Location: Kelvin Lecture Theatre **Oliver Röhrle** **Continuum-mechanical Modelling of the Musculoskeletal System**	

10:30 - 11:00	Refreshments Haslett and Marconi Rooms

11:00 - 12:30	Organ Modelling and Simulation
Location: Kelvin Lecture Theatre Chair: Giulia Luraghi	
11:00	**Use of 3D Atrial Models to Improve Signal Processing in Cardiac Electrophysiology** Alejandro Liberos, Universitat Politècnica de València
11:20	**An Automated Pipeline for Real Time Visualisation of Blood Flow During Treatment of Intracranial Aneurysms** Robin Richardson, University College London
11:35	**A Cerebral Circulation Model for *in silico* Clinical Trials of Ischaemic Stroke** Tamas Jozsa, Institute of Biomedical Engineering, University of Oxford
11:50	**Platelet Adhesion and Aggregation: Cell-resolved Simulations and *In vitro* Experiments** Britt Van Rooij, University of Amsterdam
12:05	**A Three-dimensional Mesoscopic Model of Thrombolysis** Remy Petkantchin, University of Geneva
12:20	***End of Session***

11:00 - 12:30	Machine Learning, Big Data & AI
Location: Turing Lecture Theatre Chair: Rick Stevens	
11:00	**Machine Learning Models of Brain Ageing in Health and Disease** James Cole, Kings College London
11:20	**Automated Parameter Tuning for Living Heart Human Model using Machine Leaning and Multiscale Simulations** Clint Davis-Taylor, Dassault Systemes
11:35	**Combining Molecular Simulation and Machine Learning to INSPIRE Improved Cancer Therapy** David Wright, University College London
11:50	**Safety, Reproducibility, Performance: Accelerating Cancer Drug Discovery with ML and HPC Technologies** Amanda Minnich, Lawrence Livermore National Laboratory
12:05	**Deep Medical Image Analysis with Representation Learning and Neuromorphic Computing** Fangfang Xia, Argonne National Laboratory
12:20	**Deep Learning in Cancer Drug Response Prediction** Rick Stevens, Argonne National Laboratory
12:35	***End of Session***

11:00 - 12:30	Uncertainty Quantification
Location: Watson Watt Room Chair: Alfons Hoekstra	
11:00	**Sensitivity and Uncertainty Analysis of Cardiac Cell Models with Gaussian Process Emulators** Richard Clayton, University of Sheffield
11:20	**Pathological Test for Cardio/Cerebrovascular Diseases: Platelets Dynamics and Approximate Bayesian Computation** Ritabrata Dutta, University of Warwick
11:35	**Use of a Gaussian Process Emulator and 1D Circulation Model to Characterize Cardiovascular Pathologies and Guide Clinical Treatment** Alberto Marzo, University of Sheffield
11:50	**Uncertainty Quantification and the Calibration of Numerical Models** Peter Challenor, University of Exeter
12:10	***End of Session***

12:30 – 13:30	***Lunch*** ***Haslett and Marconi Rooms***

13:30 – 15:30	Organ Modelling and Simulation
Location: Kelvin Lecture Theatre Chair: Hector Martinez-Navarro	
13:30	**Multi-scale, Patient-specific Modelling Approaches to Predict Neointimal Hyperplasia Growth in Femoro-popliteal Bypass Grafts** Mirko Bonfanti, University College London
13:50	***In vivo*, *in silico*, *in vitro* Patient-specific Analysis of the Haemodynamics of a Type-B Aortic Dissection** Gaia Franzetti, University College London
14:05	**AngioSupport: an Interactive Tool to Support Coronary Intervention** Bettine Van Willigen, LifeTec Group
14:20	**Developments for the Efficient Self-coupling of HemeLB** Jon McCullough, University College London
14:35	**Interplay Between Thermal Transfers and Degradation of the Bronchial Epithelium During Exercise** Cyril Karamaoun, Université Côte d'Azur
14:50	**Simulation of the Thrombectomy Procedure in a Realistic Intracranial Artery** Giulia Luraghi, Politecnico di Milano
15:05	***End of Session***

13:30 – 15:30	From Quantum AI to the Virtual Human
Location: Turing Lecture Theatre Chair: Peter Love	
13:30	**Introduction** Peter Love, Tufts University
13:45	**Excited-State Dynamics: Linking Classical and Quantum Approaches** Prineha Narang, Harvard University (Remote Presentation)
14:15	**Quantum computing using continuous-time evolution** Vivien Kendon, Durham University
14:45	**Quantum Inspired Optimisation: Transforming Healthcare Imaging using Quantum-accelerated Algorithms** Anita Ramanan & Frances Tibble, Microsoft
15:05	**Atos Quantum Learning Machine: Heading Towards a Quantum-accelerated Life Science** Andy Grant, Atos
15:20	**Quantum AI to the Virtual Human: Where's the Virtual Human?** Peter V. Coveney, University College London
15:35	***End of Session***

13:30 - 15:30	Genomics
Location: Watson Watt Room Chair: Nikolas Maniatis	
13:30	**Reconstructing Mutational Histories of Oesophageal Cancer** Maria Secrier, University College London
13:50	**CDK11 Binds Chromatin and mRNAs of Replication Dependent Histones Regulating Their Expression.** Igor Ruiz de Los Mozos, Francis Crick Institute
14:10	**The Power of High-resolution Population-specific Genetic Maps to Dissect the Genetic Architecture of Complex Diseases: Type 2 Diabetes as an Example** Nikolas Maniatis, University College London
14:30	**Genetic Fine-mapping and Targeted Sequencing to Investigate Allelic Heterogeneity and Molecular Function at Genomic Disease Susceptibility Loci for Type 2 Diabetes** Toby Andrew, Imperial College London
14:50	**Pathway Analysis Reveals Genetic Regulation of Mitochondrial Function and Branched-chain Amino Acid Catabolism in Type 2 Diabetes** Hannah Maude, Imperial College London
15:00	**Trans-ethnic Colocalization: A Novel Approach to Assess the Transferability of Trait Loci Across Populations** Karoline Kuchenbaeker, University College London
15:10	**The Genetic Architecture of T-wave Morphology Restitution** Julia Ramírez, Queen Mary University of London
15:20	**Genetic Architecture of QT Dynamics and Resting QT in the General Population** Stefan van Duijvenboden, University College London
15:30	***End of Session***

15:30 - 17:00	**Refreshments** **Haslett and Marconi Rooms**
	Poster Presentations **Haslett Room**

Poster Presentations

Genomics

Julie Cigrang, Hannah Maude, Winston Lau, Nikolas Maniatis, Filippo Tamanini and Toby Andrew
Functional and in Silico Analysis of the Novel Identified Type 2 Diabetes Susceptibility Locus FGF14 and the Associated Dysregulation of Propionyl-coA Carboxylase (PCCA) Gene Expression.

Kate Mackie, Hannah Maude, Winston Lau, Nikolas Maniatis, Filippo Tamanini and Toby Andrew
An Investigation into the Role of the ACAD11 Disease Susceptibility Locus in Conferring Risk of Type 2 Diabetes

Dhryata Kamdar, Winston Lau, Nikolas Maniatis and Toby Andrew
eQTL Co-Localisation Using Transcriptome Datasets from Different Tissues on a Type 2 Diabetes Susceptibility Locus, MAPK8-IP3

Shirin Saverimuttu, Barbara Kramarz and Ruth Lovering
Describing the Role of microRNAs in Alzheimer's Disease Using a Bioinformatics Approach

Machine Learning, Big Data and AI

Adrià Pérez Culubret, Pablo Herrera Nieto, Stefan Doerr and Gianni De Fabritiis
A Multi-Armed Bandit Framework for Adaptive Sampling in Molecular Simulations

Peter Zinterhof and Yu Wang
Getting More for Less: Semi-Supervised Learning Approach for Medical Image Segmentation

Molecular Medicine

David Chisholm, Valerie Affleck, Josh Hughes, Dan Callaghan, Andy Whiting and Carrie Ambler
Small Molecule Photosensitisers for Light-Activated Cell Death

Mabel Wong, Xiaofeng Liu, Richard Taylor, Terry Baker and Jonathan Essex
A Loopy Study of the Antibody-Antigen Interface

Giulio Mattedi, Francesca Deflorian, Jonathan Mason, Chris de Graaf and Francesco Gervasio
Understanding Ligand Binding Selectivity in a Prototypical GPCR Family

Grigor Arakelov, Peter Coveney and Karen Nazaryan
***In silico* Study of the Pyrin Inflammasome Macromolecular Complex Formation.**

Organ Modelling and Simulation

Tim van den Boom, Bettine van Willigen, Marco Stijnen and Frans van de Vosse
Pulse Wave Propagation Modelling with Reduced Complexity

Sathyavani Malyala, Richard Clayton and Alberto Marzo
Modelling of Electrophysiology of the Heart and Treatment of Ventricular Fibrillation

Mattia d'Alessi and Marco Stijnen
The Addition of Compliance and Deformation of Vessel Walls in 3D CFD Simulations

Alexandra Buess
The Influence of Asymmetry in Health and Disease on Gaseous Transport and Exchange in the Human Lungs: A Model Approach

The Role of Theory in Modelling and Simulation

Rukmankesh Mehra and Kasper Planeta Kepp
Molecular Dynamics of Aβ Peptide: Hydrophobic Exposure Is a Significant Event at Low Water Potential

Antonija Kuzmanic and Francesco Gervasio
Exploring Cryptic Pockets Formation in Targets of Pharmaceutical Interest

Ella van de Pol and Marco Stijnen
Possibilities of 3D-1D Coupled Models in Hemodynamic Simulations

Chiara Fais, Elizabeth M. Grimsey, Robert L. Marshall, Vito Ricci, Maria Laura Ciusa, Al Ivens, Giuliano Malloci, Paolo Ruggerone, Attilio V. Vargiu and Laura J.V. Piddock
Chlorpromazine and Amitriptyline Are Substrates and Inhibitors of the AcrB Multidrug Efflux Pump

Alessandro Crnjar and Carla Molteni
Environment Effects on a Potential Trans-Cis Molecular Switch for Opening the Ion Channel of the Serotonin-Activated 5-HT3 Receptor

Alireza Meghdadi, Marcus Caine, Stephen Jones, Venisha Patel, Lorenzo Capretto, Andrew Lewis and Dario Carugo
A Parametric in Silico Investigation for Characterisation of Drug-Eluting Bead (DEB) Trajectory Distributions

Education, Training and Public Engagement

Xan Wesolowski, UCL
Cigarettes vs E-Cigarettes: The Effect on the Oral Microbiome

Julio Revilla Navarro
Microbiome Diversity of Tattooed and Non-Tattooed Skin

Dan Smaje
A Comparison of the Microbial Diversity in Mass-Produced and Artisan Cheeses

Full Programme

Thursday 26th September

09:00 - 09:45	Keynote Address
Location: Kelvin Lecture Theatre **Andrew Hopkins** **How Machines can Design Drugs**	

09:45 - 10:15	Refreshments Haslett and Marconi Rooms

10:15 - 12:00	Molecular Medicine
Location: Kelvin Lecture Theatre Chair: Herman Van Vlijmen	
10:15	**On the Faithfulness of Molecular Mechanics Representations in Multi-scale Free Energy Simulations** Gerhard König, ETH Zurich
10:35	**Entropy Estimation Methods in Ensemble End-point Binding Free Energy Simulations** David Wright, University College London
10:50	**Rapid, Qualitative Prediction of Antimicrobial Resistance by Alchemical Free Energy Methods** Philip Fowler, University of Oxford
11:05	**Opportunities and Challenges for Free Energy Calculations in Drug Design** Christina Schindler, Merck Healthcare KGaA
11:25	**Accurate and Precise Predictions of the Influence of Salt Concentration on the Conformational Stability and Membrane-Binding Modes of Multifunctional DNA Nanopores using Ensemble-Based Coarse-Grained Molecular Dynamics** Katya Ahmad, University College London
11:40	**The Role of Water in Mediating Biomolecular Binding: From Water Locations to Their Impact on Binding Affinity** Jonathan Essex, University of Southampton
12:00	***End of Session***

10:15 - 12:10	Machine Learning, Big Data & AI
Location: Turing Lecture Theatre Chair: Fangfang Xia	
10:15	**AI for Big Science** Tony Hey, Science Technology Facilities Council (STFC)
10:35	**Applying Artificial Intelligence in Drug Design** Ola Engkvist, AstraZeneca
10:50	**The Convergence of HPC and AI for Healthcare on Intel® Based Supercomputers** Valeriu Codreanu, SURFsara
11:05	**Accelerating Deep Learning Adoption in Biomedicine with the CANDLE Framework** Justin Wozniak, Argonne National Laboratory
11:20	**The Influence of DNA Sequence-Derived Features Across the 'omics Scales** Gregory Parkes, University of Southampton
11:35	**Predicting ICU Readmission with Context-Enriched Deep Learning** Rafael Zamora-Resendiz, Lawrence Berkeley National Laboratory
11:50	**GuacaMol: Benchmarking Models for De Novo Molecular Design** Marwin Segler, BenevolentAI
12:10	***End of Session***

10:15 - 12:00	Regulatory Science and *in silico* Trials
Location: Watson Watt Room Chair: Alfons Hoekstra and Marco Viceconti	
10:15	***In silico* Trials and Drug Approval Process: Where are we?** Flora Musuamba Tshinanu, Federal Agency for Medicines and Health Products
10:35	**InSilc: an *in silico C*linical Trials Platform for Advancing BVS Design and Development** Georgia Karanasiou, FORTH
10:50	**Credibility of UISS-TB Modelling and Simulation Framework** Francesco Pappalardo, University of Catania
11:05	**Modelling Bone at the Tissue Scale: the Missing Link Between Drug Design and Clinical Outcome** Marco Viceconti, University of Bologna
11:20	***In silico* Trials for Drug Tracing the Effects of Sarcomeric Protein Mutations Leading to Familial Cardiomyopathy- SILICOFCM Project** Nenad Filipovic, Bioengineering Research and Development Center BioIRC
11:35	**INSIST: *In silico* Trials for Acute Ischemic Stroke.** Alfons Hoekstra, University of Amsterdam
11:50	***End of Session***

12:00 – 13:00	***Lunch*** ***Haslett and Marconi Rooms***

13:00 – 15:00	Molecular Medicine
Location: Kelvin Lecture Theatre Chair: Peter V Coveney	
13:00	**Computational Molecular Design in Pharmaceutical Drug Discovery** Katharina Meier, Bayer AG
13:20	**Accurate, Precise and Reliable Binding Affinity Predictions for G Protein Coupled Receptors** Shunzhou Wan, University College London
13:35	**An Ensemble-Based Steered Molecular Dynamics (SMD) Workflow that Predicts the Residence Time of A2A Receptor Ligands** Andrew Potterton, University College London
13:50	**Understanding Induced Conformational Plasticity in G-Protein Coupled Receptors Selective Pathway Activation** Silvia Acosta Gutierrez, University College London
14:05	**Clustering Analysis of Synthetic Retinoid Docking** Jason Clark, Durham University
14:20	**Analysis of Mechanotransduction Dynamics During Combined Mechanical Stimulation and Modulation of Mechanotransduction Cascade Uncover Hidden Information Within the Signalling Noise** Aban Shuaib, NSIGNEO Institute for *in silico* Medicine, University of Sheffield
14:35	**Adaptive Sampling for Alchemical Free Energy Calculations and Applications for Drug Design** Hannah Bruce Macdonald, Memorial Sloan Kettering Cancer Center
14:50	***End of Session***

13:00 – 15:00	Innovation in Modern Biotechnology
Location: Turing Lecture Theatre Chair: Herman Van Vlijmen	
13:00	**ELEM Biotech – The Virtual Humans Factory** Mariano Vazquez, ELEM Biotech
13:20	**Balancing Research and Production: Alces Flight's Take on Building up Commercial Compute** Cristin Merritt, Alces Flight
13:40	**The Rise of PlayMolecule** Raimondas Galvelis, Acellera
14:00	**InSilicoTrials.Com: A Cloud-Based Platform to Drive Technology Transfer of Modeling and Simulation Tools across Healthcare** Luca Emili, InSilicoTrials
14:20	**Panel Discussion**
15:00	***End of Session***

13:00 - 15:00	Education, Training and Public Engagement
Location: Watson Watt Room Chair: Andrea Townsend-Nicholson	
13:00	**Reflections on Educating and Engaging New Communities of Practice with High Performance Computing Through the Integration of Teaching and Research** Andrew Townsend-Nicholson, University College London
13:20	**Computational Biomedicine –Interdisciplinary Training for the Clinician Scientists of the Future** Benny Chain, University College London
13:40	**Promoting a Research-Based Education through Undergraduate Research Experience for Students** Othmane Bouhali, Texas A&M University
13:55	**AI for Science** Rick Stevens, Argonne National Laboratory
14:15	**Integrating Computational Biology and Soil Metagenomics: an Undergraduate study** Mariana Pereira da Costa, University College London
14:30	**Panel Discussion**
15:00	***End of Session***

15:00 - 15:30	Refreshments Haslett and Marconi Rooms

15:30 - 17:00	Molecular Medicine
Location: Kelvin Lecture Theatre Chair: Christina Schindler	
15:30	***In Silico* Search for Endogenous Inhibitors of Protein Misfolding** Donald Weaver, Krembil Research Institute
15:50	**The Influence of Base Pair Tautomerism on Single Point Mutations in Aqueous DNA** Alexander Gheorghiu, University College London
16:05	**Monte Carlo Modelling of a VARIAN 2300C/D Photon Accelerator** Othmane Bouhali, Texas A&M University
16:20	**Molecular Organization of Tight Junction Protein Strands: Molecular Dynamics Simulation of the Self-Assembly of Extracellular Domain Particles of Claudin 1** Eleni Fitsiou, Lancaster University
16:35	***End of Session***

15:30 - 17:00	Multiscale Modelling
Location: Turing Lecture Theatre Chair: Derek Groen	
15:30	**Dynamics of Nonequilibrium Self-Assembly Through Reaction-Diffusion Simulations** Margaret Johnson, Johns Hopkins University
15:50	**Predictions of Age-specific Hip Fracture Incidence in Elderly British Women based on a Virtual Population Model** Pinaki Battacharya, University of Sheffield
16:05	**Suitability of Scaled Generic Musculoskeletal models in Predicting Longitudinal Changes in Joint Contact Forces in Children with Juvenile Idiopathic Arthritis** Claude Hayford, University of Sheffield
16:20	**Refining Low-Resolution Cryo-EM Structures with Bayesian Inference Driven Integration of Multiscale Simulations** Arvind Ramanthan, Argonne National Laboratory
16:35	***End of Session***

15:30 - 17:00	Cloud & High Performance Computing
Location: Watson Watt Room Chair: Marco Verdicchio	
15:30	**Advancing Personalized Healthcare with High-Performance Cloud Computing for the Living Heart Project** Wolfgang Gentzsch, UberCloud
15:50	**Large Scale Binding Affinity Calculations on Commodity Compute Clouds** Stefan Zasada, EnsembleMD Ltd
16:05	**Processing Complex Medical Workflows in the EurValve Environment** Piotr Nowakowski, ACC Cyfronet AGH, Kraków, Poland
16:20	**The HemeLB Offloader** Terry Sloan, EPCC
16:35	**Structural Biology in the Clouds: Past, Present and Future** Alexandre Bonvin, Utrecht University
16:55	***End of Session***

Full Programme

Friday 27th September

09:00 – 09:45	Keynote Address
Location: Kelvin Lecture Theatre **Anne Robertson** **Identifying Physical Causes of Failure in the Cerebral Aneurysm Wall**	

09:45 – 10:15	Refreshments Haslett and Marconi Rooms

10:15 – 12:00	Organ Modelling and Simulation
Location: Kelvin Lecture Theatre Chair: Claudia Mazza	
10:15	**The Role of Haemodynamics and Peripheral Vasculature in Vessel Constriction After Aneurysm Treatment with Flow-Diverter Stents** Alberto Marzo, University of Sheffield
10:35	**The Effect of Gender and Endocardial Detail on Anatomically Normal Human Heart Electrophysiology** Jazmin Aguado-Sierra, Barcelona Supercomputing Center
10:50	**Connecting Arterial Blood Flow to Tissue Perfusion for In Silico Trials of Acute Ischaemic Stroke** Raymond Padmos, Institute for Informatics, University of Amsterdam
11:05	**A Novel Multi-Scale, Multi-Compartment Model of Oxygen Transport – Towards In-Silico Clinical Trials in the Entire Human Brain** Yun Bing, University of Oxford
11:20	**Delivering the CT2S Computational Workflow Directly to the Clinic** Andrew Narracott, University of Sheffield
11:35	**A Finite Element Investigation of the Positioning of Arabin® Cerclage Pessary in the Prevention of Spontaneous Preterm Birth** Xinshan Li, University of Sheffield
11:55	***End of Session***

10:15 - 12:00	Multiscale Modelling
Location: Turing Lecture Theatre Chair: Derek Groen	
10:15	**Coupling Scheme for a High-Performance Multiscale Blood Flow Simulation Workflow** Gábor Zavodszky, University of Amsterdam
10:35	**In Silico Assessment of Cardio-protection by Therapeutic Hypothermia** Sanjay Kharche, Lawson Health Research Institute, University of Western Ontario
10:50	**HPC Simulations for in Silico Drug Testing in Humans: Therapeutic Strategies in Acute Myocardial Ischemia** Hector Martinez-Navarro, University of Oxford
11:05	**Is Insulating Border Necessary for Human Sinoatrial Node Spontaneous Activity?** Sanjay Kharche, Lawson Health Research Institute, University of Western Ontario
11:20	**Multiscale Modeling of RAS on Cellular Membranes** Dwight Nissley, Frederick National Laboratory for Cancer Research and Frederick Streitz, Lawrence Livermore National Laboratory
11:40	***End of Session***

10:15 - 12:00	Cloud & High Performance Computing
Location: Watson Watt Room Chair: Marco Verdicchio	
10:15	**Integrating HPC and Deep Learning in Converged Workflows** Andy Grant, Atos
10:30	**Supporting advanced HPC/HTC scientific workloads with QCG services** Tomasz Piontek, PSNC
10:45	**Digital Blood in Massively Parallel CPU/GPU Systems for the Study of Platelets Deposition** Christos Kotsalos, University of Geneva
11:00	**Parallelising Image Registration and the HPC Porting Journey** Phil Tooley, The Numerical Algortihms Group, University of Sheffield
11:15	**Secure Processing of Sensitive Data on Shared HPC Systems** Narges Zarrabi, SURFsara
11:30	**Zettascale Computing on an Exascale Platform** Shantenu Jha, Rutgers University
11:45	**The POP Centre of Excellence – Improving Parallel Codes** Craig Lucas, The Numerical Algortihms Group, University of Sheffield
12:00	***End of Session***

12:00 – 13:00	***Lunch*** ***Haslett and Marconi Rooms***

13:00 – 15:00	**Role of Theory in Modelling and Simulation**
Location: Kelvin Lecture Theatre Chair: Erik Lindahl	
13:00	**An Agent-Based Model for Investigation of Immunological Synapse Patterns** Michael Dustin, University of Oxford
13:20	**Simulation and Experimental Evidence for the Decrease of Platelet Margination with an Increase in Volume Fraction of Stiffened Red Blood Cells in Flow** Benjamin Czaja, University of Amsterdam
13:40	**From Genome to Personalised Medicine: Cancer Treatment and Discovery of Novel Variants in Qatar** Shunzhou Wan, University College London
13:55	**The Noisy Physics of Protein Signalling: Global Low Frequency Protein Motions in Allosteric Binding** Tom McLeish, University of York
14:15	**Panel Discussion**
15:00	***End of Session***

13:00 – 15:00	**Machine Learning applications in Oncology** followed by **Immunology**
Location: Turing Lecture Theatre Chair: Eric Stahlberg and Tim Elliott	
13:00	**Artificial Intelligence Solutions to Modernize Cancer Surveillance and Optimize Population-Level Cancer Outcomes** Georgia Tourassi, Oak Ridge National Laboratory
13:30	**Towards Personalised Cancer Prevention: The Digital Cancer Precision Prevention Initiative** Mari Nygård, Cancer Registry of Norway
14:00	**Immune Cell Dynamics & Control of Persistent Virus Infection** Becca Asquith, Imperial College London
14:20	**Control of T Cell Responses by Accessory Receptors Revealed by Phenotypic Modelling** Omer Dushek, University of Oxford
14:40	**Application of Artificial Neural Networks to Infer Pharmacological Molecular-Level Mechanisms of Drug Evoked Clinical Responses** Jonathan Wagg, Roche
15:00	***End of Session***

13:00 - 15:00	Imaging & Visualisation
Location: Watson Watt Room Chair: Peter V Coveney	
13:00	**Accelerating Medical Imaging on Multi-core Platforms** Abbes Amira, Qatar University
13:20	**Improved Data Analysis with Virtual and Augmented Reality** Thomas Odaker, Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities
13:40	**Automatic Cerebral Aneurysm Segmentation Using Contourlet Transform and Hidden Random Field Model Template** Abbes Amira, Qatar University
13:55	**Animating the Virtual Human: Applying Movie-industry Tools and Techniques to Data Visualization** Guillermo Marin, Barcelona Supercomputing Center
14:15	**Panel Discussion**
15:00	***End of Session***

15:00 - 15:30	Refreshments Haslett and Marconi Rooms

15:30 - 16:15	Keynote Address
Location: Kelvin Lecture Theatre **William L. Jorgensen** **Computer-Guided Efficient Discovery of Potent Enzyme Inhibitors**	

16:15 - 16:30	Sano Project
Location: Kelvin Lecture Theatre Marian Bubak	

16:30 - 17:00	Closing Remarks and Poster Prize
Location: Kelvin Lecture Theatre Peter V. Coveney	