



## Full Programme

### Wednesday 25<sup>th</sup> September

<b>09:30 - 09:45</b>	<b>Welcome Address</b>
Location: Kelvin Lecture Theatre Peter V. Coveney	

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

<b>10:30 - 11:00</b>	<b>Refreshments</b>
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<b>11:00 - 12:30</b>	<b>Organ Modelling and Simulation</b>
Location: Kelvin Lecture Theatre Chair: Giulia Luraghi	
11:00	<b>Use of 3D atrial models to improve signal processing in cardiac electrophysiology</b> Alejandro Liberos, Universitat Politècnica de València
11:20	<b>An automated pipeline for real time visualisation of blood flow during treatment of intracranial aneurysms</b> Robin Richardson, University College London
11:35	<b>A cerebral circulation model for in silico clinical trials of ischaemic stroke</b> Tamas Jozsa, Institute of Biomedical Engineering, University of Oxford
11:50	<b>Platelet adhesion and aggregation: Cell-resolved simulations and In vitro experiments</b> Britt Van Rooij, University of Amsterdam
12:05	<b>A Three-dimensional Mesoscopic Model of Thrombolysis</b> Remy Petkantchin, University of Geneva
12:20	<b>End of Session</b>

<b>11:00 - 12:30</b>		<b>Machine Learning, Big Data &amp; AI</b>
Location: Turing Lecture Theatre		
Chair: Rick Stevens		
11:00	<b>Machine learning models of brain ageing in health and disease</b>	James Cole, Kings College London
11:20	<b>Automated Parameter Tuning for Living Heart Human Model using Machine Learning and Multiscale Simulations</b>	Clint Davis-Taylor, Dassault Systemes
11:35	<b>Combining molecular simulation and machine learning to INSPIRE improved cancer therapy</b>	David Wright, University College London
11:50	<b>Safety, Reproducibility, Performance: Accelerating cancer drug discovery with ML and HPC technologies</b>	Amanda Minnich, Lawrence Livermore National Laboratory
12:05	<b>Deep Medical Image Analysis with Representation Learning and Neuromorphic Computing</b>	Fangfang Xia, Argonne National Laboratory
12:20	<b>Deep Learning in Cancer Drug Response Prediction</b>	Rick Stevens, Argonne National Laboratory
12:35	<b><i>End of Session</i></b>	

<b>11:00 - 12:30</b>		<b>Uncertainty Quantification</b>
Location: Watson Watt Room		
Chair: Peter V. Coveney		
11:00	<b>Sensitivity and uncertainty analysis of cardiac cell models with Gaussian process emulators</b>	Richard Clayton, University of Sheffield
11:20	<b>Pathological Test for Cardio/cerebrovascular diseases: Platelets dynamics and Approximate Bayesian computation</b>	Ritabrata Dutta, University of Warwick
11:35	<b>Use of a Gaussian process emulator and 1D circulation model to characterize cardiovascular pathologies and guide clinical treatment</b>	Alberto Marzo, University of Sheffield
11:50	<b>Safety, Reproducibility, Performance: Accelerating cancer drug discovery with ML and HPC technologies</b>	Peter Challenor, University of Exeter
12:10	<b><i>End of Session</i></b>	

<b>12:30 – 13:30</b>	<b>Lunch</b>
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<b>13:30 - 15:30</b>		<b>Organ Modelling and Simulation</b>
Location: Kelvin Lecture Theatre		
Chair: Hector Martinez-Navarro		
13:30	<b>Multi-scale, patient-specific modelling approaches to predict neointimal hyperplasia growth in femoro-popliteal bypass grafts</b> Mirko Bonfanti, University College London	
13:50	<b>In vivo, in silico, in vitro patient-specific analysis of the haemodynamics of a Type-B Aortic Dissection</b> Gaia Franzetti, University College London	
14:05	<b>AngioSupport: an interactive tool to support coronary intervention</b> Bettine Van Willigen, LifeTec Group	
14:20	<b>Developments for the Efficient Self-coupling of HemeLB</b> Jon McCullough, University College London	
14:35	<b>Interplay between thermal transfers and degradation of the bronchial epithelium during exercise</b> Cyril Karamaoun, Université Côte d'Azur	
14:50	<b>Simulation of the thrombectomy procedure in a realistic intracranial artery</b> Giulia Luraghi, Politecnico di Milano	
15:05	<b><i>End of Session</i></b>	

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

<b>13:30 - 15:30</b>		<b>Genomics</b>	
Location: Watson Watt Room			
Chair: Nikolas Maniatis			
13:30	<b>Reconstructing mutational histories of oesophageal cancer</b>	Maria Secrier, University College London	
13:50	<b>CDK11 binds chromatin and mRNAs of replication dependent histones regulating their expression.</b>	Igor Ruiz de Los Mozos, Francis Crick Institute	
14:10	<b>The power of high-resolution population-specific genetic maps to dissect the genetic architecture of complex diseases: Type 2 Diabetes as an example</b>	Nikolas Maniatis, University College London	
14:30	<b>Genetic fine-mapping and targeted sequencing to investigate allelic heterogeneity and molecular function at genomic disease susceptibility loci for Type 2 Diabetes</b>	Toby Andrew, Imperial College London	
14:50	<b>Pathway analysis reveals genetic regulation of mitochondrial function and branched-chain amino acid catabolism in Type 2 Diabetes</b>	Hannah Maude, Imperial College London	
15:00	<b>Trans-ethnic colocalization: A novel approach to assess the transferability of trait loci across populations</b>	Karoline Kuchenbaecker, University College London	
15:10	<b>The Genetic Architecture of T-wave Morphology Restitution</b>	Julia Ramírez, Queen Mary University of London	
15:20	<b>Genetic architecture of QT dynamics and resting QT in the general population</b>	Stefan van Duijvenboden, University College London	
15:30	<b><i>End of Session</i></b>		

<b>15:30 - 17:00</b>	<b>Refreshments</b>		
	<b>Poster Presentations</b>		



## 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 bioinformatic 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 A $\beta$  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-HT<sub>3</sub> 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**



## Full Programme

**Thursday 26<sup>th</sup> September**

<b>09:00 - 09:45</b>	<b>Keynote Address</b>
Location: Kelvin Lecture Theatre	
<b>Andrew Hopkins</b>	
<b>How machines can design drugs</b>	

<b>09:45 - 10:15</b>	<b>Refreshments</b>
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<b>10:15 - 12:00</b>	<b>Molecular Medicine</b>
Location: Kelvin Lecture Theatre	
Chair: Herman Van Vlijmen	
10:15	<b>On the faithfulness of molecular mechanics representations in multi-scale free energy simulations</b> Gerhard König, ETH Zurich
10:35	<b>Entropy estimation methods in ensemble end-point binding free energy simulations</b> David Wright, University College London
10:50	<b>Rapid, qualitative prediction of antimicrobial resistance by alchemical free energy methods</b> Philip Fowler, University of Oxford
11:05	<b>Opportunities and challenges for free energy calculations in drug design</b> Christina Schindler, Merck Healthcare KGaA
11:25	<b>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</b> Katya Ahmad, University College London
11:40	<b>The Role of Water in Mediating Biomolecular Binding: From Water Locations to Their Impact on Binding Affinity</b> Jonathan Essex, University of Southampton
12:00	<b><i>End of Session</i></b>

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

<b>10:15 - 12:00</b>		<b>Regulatory Science and <i>in silico</i> Trials</b>	
Location: Watson Watt Room			
Chair: Alfons Hoekstra and Marco Viceconti			
10:15	<b>In silico trials and drug approval process: where are we?</b>	Flora Musuamba Tshinanu, Federal Agency for Medicines and Health Products	
10:35	<b>InSilc: an in silico clinical trials platform for advancing BVS design and development</b>	Georgia Karanasiou, FORTH	
10:50	<b>Credibility of UISS-TB modelling and simulation framework</b>	Francesco Pappalardo, University of Catania	
11:05	<b>Modelling bone at the tissue scale: the missing link between drug design and clinical outcome</b>	Marco Viceconti, University of Bologna	
11:20	<b>In Silico trials for drug tracing the effects of sarcomeric protein mutations leading to familial cardiomyopathy- SILICOFCM project</b>	Nenad Filipovic, Bioengineering Research and Development Center BioIRC	
11:35	<b>INSIST: In-Silico Trials for Acute Ischemic Stroke.</b>	Alfons Hoekstra, University of Amsterdam	
11:50	<b>End of Session</b>		

<b>12:00 – 13:00</b>	<b>Lunch</b>
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<b>13:00 - 15:00</b>	<b>Molecular Medicine</b>
Location: Kelvin Lecture Theatre	
Chair: Peter V Coveney	
13:00	<b>Computational Molecular Design in Pharmaceutical Drug Discovery</b> Katharina Meier, Bayer AG
13:20	<b>An Ensemble-Based SMD Workflow that Predicts the Residence Time of A2A Receptor Ligands</b> Andrew Potterton, University College London
13:35	<b>Clustering analysis of synthetic retinoid docking</b> Jason Clark, Durham University
13:50	<b>Analysis of mechanotransduction dynamics during combined mechanical stimulation and modulation of mechanotransduction cascade uncover hidden information within the signalling noise</b> Aban Shuaib, NSIGNEO Institute for in silico Medicine, University of Sheffield
14:05	<b>Understanding induced conformational plasticity in G-protein coupled receptors selective pathway activation</b> Silvia Acosta Gutierrez, University College London
14:20	<b>Quantitative Evaluation of Bioisosteres in Drug Design</b> Alya Arabi, Zayed University
14:35	<b>Adaptive sampling for alchemical free energy calculations and applications for drug design</b> Hannah Bruch Macdonald, Memorial Sloan Kettering Cancer Center
14:50	<b>End of Session</b>

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

<b>13:00 - 15:00</b>		<b>Education, Training and Public Engagement</b>
Location: Watson Watt Room		
Chair: Andrea Townsend-Nicholson		
13:00	<b>Reflections on educating and engaging new communities of practice with high performance computing through the integration of teaching and research</b> Andrew Townsend-Nicholson, University College London	
13:20	<b>Computational biomedicine –interdisciplinary training for the clinician scientists of the future</b> Benny Chain, University College London	
13:40	<b>Promoting a Research-Based Education through Undergraduate Research Experience for Students</b> Othmane Bouhali, Texas A&M University	
13:55	<b>AI for Science</b> Rick Stevens, Argonne National Laboratory	
14:15	<b>Panel Discussion</b>	
15:00	<b>End of Session</b>	

<b>15:00 - 15:30</b>	<b>Refreshments</b>
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<b>15:30 - 17:00</b>		<b>Molecular Medicine</b>
Location: Kelvin Lecture Theatre		
Chair: Alya Arabi (TBC)		
15:30	<b>In Silico Search for Endogenous Inhibitors of Protein Misfolding</b> Donald Weaver, Krembil Research Institute	
15:50	<b>The influence of base pair tautomerism on single point mutations in aqueous DNA</b> Alexander Gheorghiu, University College London	
16:05	<b>Monte Carlo modelling of a VARIAN 2300C/D photon accelerator</b> Othmane Bouhali, Texas A&M University	
16:20	<b>Molecular Organization of Tight Junction Protein Strands: Molecular Dynamics Simulation of the Self-Assembly of Extracellular Domain Particles of Claudin 1</b> Eleni Fitsiou, Lancaster University	
16:35	<b>End of Session</b>	

<b>15:30 - 17:00</b>		<b>Multiscale Modelling</b>
Location: Turing Lecture Theatre		
Chair: Derek Groen		
15:30	<b>Dynamics of nonequilibrium self-assembly through reaction-diffusion simulations</b>	Margaret Johnson, Johns Hopkins University
15:50	<b>Predictions of Age-specific Hip Fracture Incidence in Elderly British Women based on a Virtual Population Model</b>	Pinaki Battacharya, University of Sheffield
16:05	<b>Suitability of Scaled Generic Musculoskeletal models in Predicting Longitudinal Changes in Joint Contact Forces in Children with Juvenile Idiopathic arthritis</b>	Claude Hayford, University of Sheffield
16:20	<b>Refining low-resolution Cryo-EM structures with Bayesian inference driven integration of multiscale simulations</b>	Arvind Ramanathan, Argonne National Laboratory
16:35	<b><i>End of Session</i></b>	

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



## Full Programme

### Friday 27<sup>th</sup> September

09:00 - 09:45	Keynote Address
Location: Kelvin Lecture Theatre	
<b>Anne Robertson</b>	
<b>Identifying Physical Causes of Failure in the Cerebral Aneurysm Wall</b>	

09:45 - 10:15	Refreshments
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10:15 - 12:00	Organ Modelling and Simulation
Location: Kelvin Lecture Theatre	
Chair: Claudia Mazza	
10:15	<b>The role of haemodynamics and peripheral vasculature in vessel constriction after aneurysm treatment with flow-diverter stents</b> Alberto Marzo, University of Sheffield
10:35	<b>The effect of gender and endocardial detail on anatomically normal human heart electrophysiology</b> Jazmin Aguado-Sierra, Barcelona Supercomputing Centre
10:50	<b>Connecting Arterial Blood Flow to Tissue Perfusion for In Silico Trials of Acute Ischaemic Stroke</b> Raymond Padmos, Institute for Informatics, University of Amsterdam
11:05	<b>A novel multi-scale, multi-compartment model of oxygen transport – Towards in-silico clinical trials in the entire human brain</b> Yun Bing, University of Oxford
11:20	<b>Delivering the CT2S computational workflow directly to the clinic</b> Andrew Narracott, University of Sheffield
11:35	<b>A finite element investigation of the positioning of Arabin® cerclage pessary in the prevention of spontaneous preterm birth</b> Xinshan Li, University of Sheffield
11:55	<b>End of Session</b>

<b>10:15 - 12:00</b>		<b>Multiscale Modelling</b>	
Location: Turing Lecture Theatre			
Chair: Derek Groen			
10:15	<b>Coupling scheme for a high-performance multiscale blood flow simulation workflow</b>	Gábor Zavodszky, University of Amsterdam	
10:35	<b>In Silico Assessment of Cardio-protection by Therapeutic Hypothermia</b>	Sanjay Kharche, Lawson Health Research Institute, University of Western Ontario	
10:50	<b>HPC simulations for in-silico drug testing in humans: therapeutic strategies in acute myocardial ischemia</b>	Hector Martinez-Navarro, University of Oxford	
11:05	<b>Is insulating border necessary for human sinoatrial node spontaneous activity?</b>	Sanjay Kharche, Lawson Health Research Institute, University of Western Ontario	
11:20	<b>Multiscale Modeling of RAS on Cellular Membranes</b>	Dwight Nissley, Frederick National Laboratory for Cancer Research and Frederick Streitz, Lawrence Livermore National Laboratory	
11:40	<b><i>End of Session</i></b>		

<b>10:15 - 12:00</b>		<b>Cloud &amp; High Performance Computing</b>	
Location: Watson Watt Room			
Chair: Marco Verdicchio			
10:15	<b>Deep Learning Training and Inference for Medical Imaging on Intel® Xeon® Processor Based Supercomputers</b>	Vikram Saletore, Intel	
10:35	<b>The POP Centre of Excellence – Improving Parallel Codes</b>	Craig Lucas, The Numerical Algorithms Group, University of Sheffield	
10:50	<b>Digital Blood in Massively Parallel CPU/GPU Systems for the Study of Platelets deposition</b>	Christos Kotsalos, University of Geneva	
11:05	<b>Parallelising Image Registration and the HPC Porting Journey</b>	Phil Tooley, The Numerical Algorithms Group, University of Sheffield	
11:20	<b>Secure Processing of Sensitive Data on shared HPC systems</b>	Narges Zarrabi, SURFsara	
11:35	<b>Integrating HPC and Deep Learning in converged workflows</b>	Andy Grant, Atos	
11:55	<b><i>End of Session</i></b>		

<b>12:00 – 13:00</b>	<b>Lunch</b>
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<b>13:00 - 15:00</b>		<b>Role of Theory in Modelling and Simulation</b>
Location: Kelvin Lecture Theatre		
Chair: Erik Lindahl		
13:00	<b>An agent-based model for investigation of immunological synapse patterns</b>	Michael Dustin, University of Oxford
13:20	<b>Accurate, Precise and Reliable Binding Affinity Predictions for G Protein Coupled Receptors</b>	Benjamin Czaja, University of Amsterdam
13:40	<b>Simulation and experimental evidence for the decrease of platelet margination with an increase of stiffened red blood cells in flow</b>	Fouad Husseini, University College London
13:55	<b>The Noisy Physics of Protein Signalling: Global Low Frequency Protein Motions in Allosteric Binding</b>	Tom McLeish, University of York
14:15	<b>Panel Discussion</b>	
15:00	<b>End of Session</b>	

<b>13:00 - 15:00</b>		<b>Machine Learning applications in Oncology</b> followed by <b>Immunology</b>
Location: Turing Lecture Theatre		
Chair: TBC and Tim Elliott		
13:00	<b>Artificial Intelligence Solutions to Modernize Cancer Surveillance and Optimize Population-Level Cancer Outcomes</b>	Georgia Tourassi, Oak Ridge National Laboratory
13:30	<b>Towards personalised cancer prevention: The Digital Cancer Precision Prevention Initiative</b>	Mari Nygård, Cancer Registry of Norway
14:00	<b>Immune cell dynamics &amp; control of persistent virus infection</b>	Becca Asquith, Imperial College London
14:20	<b>Control of T cell responses by accessory receptors revealed by phenotypic modelling</b>	Omer Dushek, University of Oxford
14:40	<b>Application of Artificial Neural Networks to Infer Pharmacological Molecular-Level Mechanisms of Drug Evoked Clinical Responses</b>	Jonathan Wagg, Roche
15:00	<b>End of Session</b>	

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

<b>15:00 - 15:30</b>		<b>Refreshments</b>
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<b>15:30 - 16:15</b>		<b>Keynote Address</b>
Location: Kelvin Lecture Theatre		
<b>William L. Jorgensen</b>		
<b>Computer-Guided Efficient Discovery of Potent Enzyme Inhibitors</b>		

<b>16:15 - 16:30</b>		<b>Information on Sano Project</b>
Location: Kelvin Lecture Theatre		
Marian Bubak		

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