

CompBioMedX Kick Off Meeting Programme

Date: 13th December 2022, 10:00 - 18:30 (GMT), 11:00 - 19:30 (CET)

Locations to attend in person:

Ground Floor, G5 Nyholm Room, Chemistry Department, UCL, 20 Gordon Street, London, WC1H 0AJ

09:30	Arrival, registration, and refreshments	
Welcome & Introduction		
10:00	Welcome	Geraint Rees (UCL Vice Provost Research, Innovation & Global Engagement)
10:10	Overview	Peter Coveney (UCL)
10:20	Knowledge Exchange	Andrea Townsend-Nicholson (UCL)
Part 1: Growing the community in computational biomedicine		
10:30	Medics on HPC	Andrea Townsend-Nicholson (UCL)
10:40	Solutions in Diversity - A million ways to get it right	Cristin Merritt (Alces Flight)
10:50	The importance of models to improve the management of vascular pathologies: fighting Stroke with new tools	Ana Narata (NHS University Hospital of Southampton)
11:00	Atos Life Sciences CoE: enabling Computational Biomedicine at the Exascale	Natalia Jimenez (Atos)
11:10	<i>Refreshment break (20 minutes)</i>	
Part 2: Scientific Applications		
Cardiac		
11:30	Enabling in silico trials using multiscale modelling and simulation	Blanca Rodriguez (University of Oxford)
11:40	Extreme-scale computational modelling of the heart using Alya: Present and future	Jazmin Aguado Sierra (Barcelona Supercomputing Center)

11:50	A clinician's engagement with computational cardiology	Luis Da Rocha Lopes (NHS/UCL)
<i>Pandemics, Uncertainty Quantification and Public Engagement</i>		
12:00	UK Premiere of the CompBioMed film: <i>The Next Pandemic</i>	
12:10	Simulating the spread of COVID-19 on a regional level using FACS (and HPC)	Derek Groen (Brunel University)
12:20	Uncertainty quantification of (bio)molecular dynamics simulations	Maxime Vassaux (UCL/CNRS)
12:30	Public Engagement	Roger Highfield (Science Museum Group)
12:40	<i>Lunch break (60 minutes)</i>	
<i>Vascular</i>		
13:40	1D flow in elastic arteries: application to cerebral circulation and modelling of ischaemic stroke	Ivan Benemerito (University of Sheffield)
13:50	3D CFD modelling to refine treatment pathways for patients with cerebral aneurysms	Andy Narracott (University of Sheffield)
<i>Molecular</i>		
14:00	Addressing the challenge of drug discovery with Machine Learning and Exascale	Agastya Bhati (UCL)
14:10	Accelerating drug design with AI & simulation	Marco Klähn (AstraZeneca AB)
14:20	Automation and scaling of fragment molecular orbitals (QM) method for drug design	Alex Heifetz (Evotec UK Ltd)
14:30	Incorporating systems modelling into T cell immunogenicity methods	Tim Elliott (University of Oxford)
14:40	Accelerating and broadening antibiotic susceptibility testing using genetics, cloud computing and machine learning	Phil Fowler (University of Oxford)
14:50	Development updates on Digital Twins for cancer patients	Eric Stahlberg (The Frederick National Laboratory for Cancer Research, Maryland)
15:00	<i>Refreshment break (15 minutes)</i>	
Part 3:	<i>(i) Running at exascale and emerging exascale</i>	
15:15	Doing biomedicine on Frontier and other high-end supercomputers	Peter Coveney (UCL)

15:25	Preparing HemeLB for the ExaScale Frontier	Balint Joo (Oak Ridge National Laboratory)
15:35	ExaWorks: Building blocks and a SDK for exascale workflows	Shantenu Jha (Rutgers State University/Brookhaven National Laboratory)
<i>(ii) Hardware and co-design</i>		
15:45	Arm based hardware for HPC	Phil Ridley (AMR)
15:55	Architectures for Scalable GPU-accelerated systems	Filippo Spiga (nVIDIA)
16:05	Biomedical simulations at scale	Gerald Mathias (Leibniz Supercomputing Centre)
16:15	From cloud to exascale: new HPC services for research and education	Marco Verdicchio (SURF)
<i>(iii) Partner contributions:</i>		
16:25	Quantifying uncertainties in patient-specific heart models	Rodrigo Weber dos Santos (Federal University of Juiz de Fora)
16:35	The DiRAC HPC Facility	Mark Wilkinson (University of Leicester/DiRAC)
<i>(iv) External collaborators</i>		
16:45	Next Generation Search and Discovery of Biomedical Knowledge	Heather Bowling (Epistemic AI)
16:55	Towards a multi-scale model of molecular machines	Sarah Harris (University of Leeds)
17:05	Potential data/AI, UI/UX and other capabilities needed to support the project	Adrian Sutherland (Endava)
17:15	ARCHER2 overview	Gavin Pringle (EPCC)
17:25	Electrostatic simulations at Exascale – The beginning of a rusty journey	Timo Betke (UCL)
17:35	<i>Discussion - ALL</i>	
17:45	<i>Reception & networking</i>	
18:30	Close	