



***Day 1 – Tuesday 11<sup>th</sup> April 2017***

<b>09.15</b>	WP3/4 Meeting	WP2/5/6 Meeting
<b>10.45</b>	<i>Tea and Coffee</i>	
<b>11.15</b>	Peter V Coveney Mariano Vazquez	<b>Welcome and introduction to AHM agenda</b>
<b>11.30</b>	Peter V Coveney (UCL)	Work Package 1 - Management
<b>11.40</b>	Mariano Vazquez (BSC)	Work Package 2 – Biomedical Research Activities
<b>12.00</b>	Marc Boonstra (UvA)	Work Package 3 – Training & Dissemination
<b>12.10</b>	Gavin Pringle (UEDIN)	Work Package 4 – Innovation & Sustainability
<b>12.20</b>	Marco Verdicchio (SARA)	Work Package 5 – Resource & Infrastructure Support
<b>12.40</b>	Marco Viceconti (USFD)	Work Package 6 – Empowering Biomedical Applications
<b>13.00</b>	<i>Lunch</i>	
<b>14.00</b>	Jonas Latt (Unige)	Numerical Modeling of Red Blood Cells
<b>14.15</b>	Matt Harvey (Acellera)	Pain-free Scientific Computing with AceCloud
<b>14.30</b>	Erwin Laure (BioExcel)	BioExcel: The Centre of Excellence for Computational Biomolecular Research
<b>14.45</b>	Thanos Papakyriakou (Southampton University)	Identifying Molecular Mechanisms of Antigen Processing <i>in silico</i>
<b>15.00</b>	Adriano Henney (Avicenna Alliance)	Modeling and simulation: paving the way to predictive medicine.
<b>15.15</b>	Liesbet Gerris (VPH Institute)	Virtual Physiological Modeling and HPC
<b>15.30</b>	<i>Break/ Tea and Coffee</i>	
<b>16.00</b>	Round table discussion	
<b>17.00</b>	<b>Neil Dalchau (Microsoft Research Cambridge)</b>	<b>Mechanistic modeling of the antigen presentation machinery and immune surveillance</b>

<b>20.00</b>	Dinner (costs not included)	
<b><i>Day 2 – Wednesday 12<sup>th</sup> April 2017</i></b>		
<b>09.00</b>	<b>Cedric Notredame (Comparative Bioinformatics Group)</b>	<b>Improving the reproducibility of in-silico omics analysis with Nextflow</b>
<b>09.30</b>	Gavin Pringle (UEDIN)	Innovation Advisory Board
<b>09.45</b>	Thomas Keller (GSK)	Data Science in Support of Drug Discovery
<b>10.00</b>	Alexander Heifetz (Evotec)	From Receptors to Ligands: Industrial Approach to Computational Drug Discovery
<b>10.15</b>	Gerald Mathtias (LRZ)	Life sciences at LRZ
<b>10.30</b>	Blanca Rodriguez (e-Cardiology)	ESC working group on e-cardiology
<b>10.45</b>	<i>Break/ Tea and Coffee</i>	
<b>11.15</b>	Marco Verdicchio (SARA)	Resources and Infrastructures: addressing the computing needs of the biomedical community
<b>11.30</b>	Daan Broeder (EUDAT)	EUDAT infrastructure for research
<b>11.45</b>	Shantenu Jha (Rutgers)	Pre-Exascale High-throughput Binding Affinity Calculator (HT-BAC): Science, Scale and Scope
<b>12.00</b>	Herman van Vlijmen (Janssen)	Retrospective and prospective FEP calculations at Janssen
<b>12.15</b>	Albert Solernou (Leeds University)	Modelling Biomolecules at the Mesoscale with Fluctuating Finite Element Analysis
<b>12.30</b>	Hugo Falter (ETP4HPC)	ETP4HPC: Latest developments in HPC in Europe
<b>12.45</b>	Time for further discussions and questions.	
<b>13.00</b>	<i>Lunch</i>	
<b>14.00</b>	General Assembly	
<b>15.00</b>	GA report – confirm date and place of next AHM	
<b>15.30</b>	Meeting closed	