

COMPBIOMED2 KICK-OFF MEETING

DATE: 21ST – 23RD OCTOBER 2019

LOCATION: LRZ



Day 1 – Monday 21st October 2019 (13:00 – 17:30 pm)

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|-------------|--|---------------------|---|---|
| 13:00-13:30 | Registration | | | |
| 13:30-13:45 | Welcome and overview of CompBioMed2 project | Peter V Coveney | | |
| 13:45-14:00 | Opening Remarks | Dieter Kranzlmüller | | |
| 14:00-14:50 | Machine Learning, AI and mechanistic modelling/simulation | 14.00 | Vicente Grau, University of Oxford | |
| | | 14.10 | Herman Van Vlijmen, Janssen | |
| | | 14.20 | Philip Fowler, University of Oxford | Machine learning then molecular simulation: a hybrid modelling approach to predicting antimicrobial resistance. |
| | | 14.30 | Austin Clyde, Argonne National Lab, University of Chicago | Computational Drug Discovery at Scale |
| | | 14.40 | Katya Ahmad, UCL | IMPRESS: Integrated Modelling for affinity PRediction on ExaScale Systems |
| | | 14:50 | Raimondas Gaivallis, Acellera | |
| 15:00-15:30 | Break / Tea and Coffee | | | |
| 15:30-16:35 | Emergence of the exascale | 15.30 | Rick Stevens, Argonne (remote) | |
| | | 16:00 | Godehard Sutmann, Jülich/E-CAM | E-CAM and its relation to CompBioMed |
| | | 16:15 | Jon McCullough, UCL | Taking HemeLB towards the exascale and full-human blood flow simulations |
| | | 16:25 | Gábor Závodszy, UvA | Concept and implementation for a high-performance multi-scale thrombus formation model based on HemoCell |
| 16:35-17:00 | CompBioMed2 General Assembly (General Assembly members <i>only</i>) | | | |
| 17:00 | Tour around SuperMUC (registration required) | | | |
| 19:00 | Dinner (Newirt, Garching) | | | |

Day 2 – Tuesday 22nd October 2019 (9.00 – 17.30 pm)

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| 09:00-09:15 | Project Management, Dissemination and Innovation (Work Package 1) | WP1 leader (UCL) Emily Lumley | | |
| 09:15 – 10:15 | Research and Applications (Work Package 2) | WP2 leader (UvA) Alfons Hoekstra | | |
| 10:15 – 10:40 | Data Management and Analytics (Work Package 3) | WP3 leader (LRZ) Dieter Kranzlmüller | | |
| 10:40 – 11:10 | Break / Tea and Coffee | | | |
| 11:10 – 11:35 | Operations and Services (Work Package 4) | WP4 leader (SARA) Marco Verdicchio | | |
| 11:35 – 12:00 | Incubator Applications (Work Package 5) | WP5 leader (BSC) Mariano Vazquez | | |
| 12:00-13:00 | Lunch | | | |
| 13:00 – 12:30 | Engagement, Training and Sustainability (Work Package 6) | WP6 leader (USFD) Alberto Marzo | | |
| 13:30 – 14:30 | International Partners and Related projects | 13:30 | Shantenu Jha, Rutgers (remote) | DeepDriveMD: Deep-Learning Driven Adaptive Molecular Simulations for Protein Folding |
| | | 14:00 | Marian Bubak, Sano | |
| | | 14:05 | Guntram Berti, FocusCoE | |
| | | 14.15 | Peter Coveney, VECMA | VECMA – Verified Exascale Computing for Multiscale Applications |
| | | 14:25 | Marc Kirschner, EU-STANDS4PM | EU-STANDS4PM – A European standardization framework for data integration and data-driven <i>in silico</i> models for personalized medicine |
| 14:35 – 15:00 | Break/Tea and Coffee | | | |
| 15:00 – 16:35 | Associate Partners and additional presentations | 15:00 | Alya Arabi, Zayed University (remote) | Electric Field Effects on Point Mutations in a Realistic Model of DNA |
| | | 15:15 | Marco Stijnen, LifeTec Group | |
| | | 15:25 | Phillipe Hupé, Institut Curie | |
| | | 15:35 | Maria Bellantone, F1000 Research | |
| | | 15:45 | Mariano Vazquez, BSC | |

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| | | 16:00 | Julien Abi-Nahed, Hamad Medical Corporation (remote) | |
| | | 16:15 | Andrea Townsend-Nicholson, UCL (remote) | |
| 16:35 – 17:00 | Discussion of initial plans, objectives and deliverables | Led by UCL | | |
| 17:30 – 18:30 | Public event on Quantum Computing | | | |

| <i>Day 3 – Wednesday 23rd October 2019 (9.00 – 12.30 pm)</i> | | |
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| 09:00 – 10:00 | WP1 and 6 joint meeting | Various drinks and snacks available during meeting |
| 10:00 – 11:00 | WP2 and 5 joint meeting | |
| 11:00 – 11:30 | <i>Break</i> | |
| 11:30 – 12:30 | WP3 and 4 joint meeting | |
| 12:30-13:30 | Lunch | |