UNIVERSITY OF WARSAW | CeNT CENTRE OF NEW TECHNOLOGIES

invites to a seminar by

Dr. Alexander Schug

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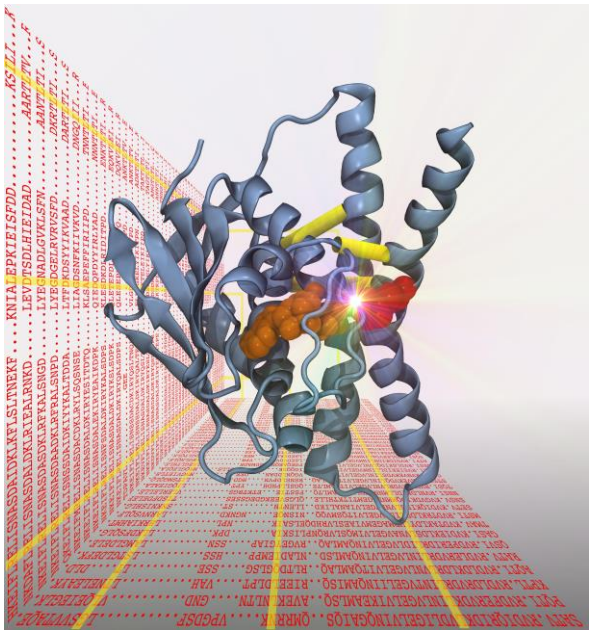
"Simulating the molecular machinery of life"

November 15th, 2018 at 12 p.m.
Venue: Centre of New Technologies, Banacha 2C, room 00.142

Host: dr hab. Joanna Sułkowska

Abstract:

Exploring the interrelationship of structure and function is crucial for the understanding of life at the molecular level. Yet despite significant progress of experimental methods, full characterization of functional cycles for biomolecules remains an ongoing challenge. Improvement of simulation techniques and rapid growth of computational resources offer a complementary option to experiments. One can use such simulations akin to an atomically resolved microscope to gain insight into the dynamical motion of biomolecules. It is also possible to enrich simulations with additional information. The increasingly ubiquitous availability of sequence information and novel statistical analysis has allowed to trace the co-evolution of residues [1], which can be exploited in structure prediction tools and is, e.g., sufficient for the blind prediction of proteins and RNA[2]. Similarly, one can use low-resolution experimental information such as SAXS data to model suitable biomolecular conformations [submitted] or compare data from simulations directly against experimental measurements such as smFRET data [3].



References

[1] Weigt M et al., Proc Nat Acad Sci USA (2009) 106, 67-72; Schug A et al., PNAS USA (2009); F. Morcos et al., PNAS (2011) 108, E1293-E1301

[2] Dago A et al., Proc Nat Acad Sci USA (2012), 109: E1733-42; E. De Leonardis et al., Nucleic acids research (2015); M. Figliuzzi et al., MBE (2016); G. Uguzzoni et al., PNASUSA (2017)

[3] I . Reinartz et al., J Chem Phys (2018)

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