CFEL SCIENCE

SEMINAR

17th April 2019 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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Molecular modelling, not just for vegans

Imagine you are a chemist who has been sentenced to life in a bioinformatics building and told that what you do is called molecular modelling. This could mean modelling a half a dozen atoms in excrutiating quantum mechanical detail or doing colloid calculations on toothpaste. There are more interesting problems which often come down to optimisation issues - sometimes discrete, sometimes continuous and sometimes discrete masquerading as continous. Can one take molecules with different sizes, but obvious similarities and find an optimal superposition? Force fields are holy objects, but can you treat atomic parameters as something to be optimised by gradient-based methods? Given some model for free energy, can you treat a biological sequence (a discrete object) as something to be optimised by continuous methods? This talk is guaranteed free of machine learning, artificial intelligence and perhaps any intelligence.

Host: Robin Santra – CFEL-DESY Theory Division