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Multiscale Computational Modelling in the field of 3R Animal Protection

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Qualitative, cartoon-based understanding of physiological processes is not sufficient and needs to be taken to a deeper, quantitative (computational) level. Two types of computational models, namely statistical & mechanistic models, can be used to predict subcellular, cellular and supracellular phenomena in silico. This talk will mainly focus on mechanistic models. A simulation of a large number of parameter combinations may lead to a reduction in the number of necessary experiments. However, experimental data from in vitro and in vivo experiments are necessary to adjust the parameters of computer models. Relatively recently established, so called population-based compartmental modeling will be presented as a promising tool to predict and partially replace pharmacological/genetical perturbations. Examples from cardiac and neuronal physiology will be described to show how population-based computational modeling enables studies of the functional impact of intercellular ion channel variability. In addition, morphological modeling will be mentioned as a useful complementary approach to traditional compartmental modeling of electrophysiological data in neurobiology. In combination, morphological and compartmental modeling facilitates generalization of computational predictions to any morphology and supports the search for universal principles valid across different species and cell types. Multi-objective Pareto optimality will be discussed as a helpful guiding principle to address the degeneracy of model parameters. Pareto optimality might help identify the subpopulations of models that strike the best balance between their economy and functionality. This approach could potentially reduce the high-dimensional parameter space of models to geometrically simple low-dimensional manifolds.

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