

EU-MORNET

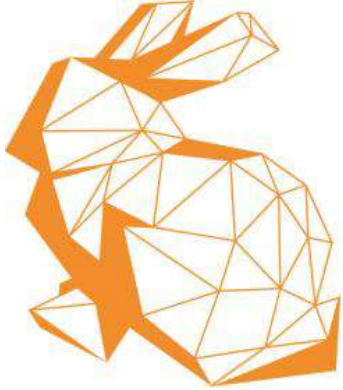
European Network for Model Reduction ★★



Multi-scale modelling of Biological Systems

Ruxandra Bărbulescu





EU-MORNET
European Network for Model Reduction ★★



CONTENTS

Systems Biology

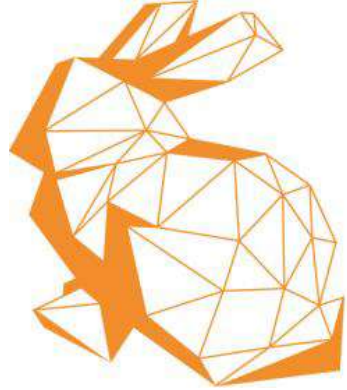
The MMM

Abstraction levels of hierarchical biological organization

Multi-scale methods in modelling of biological systems

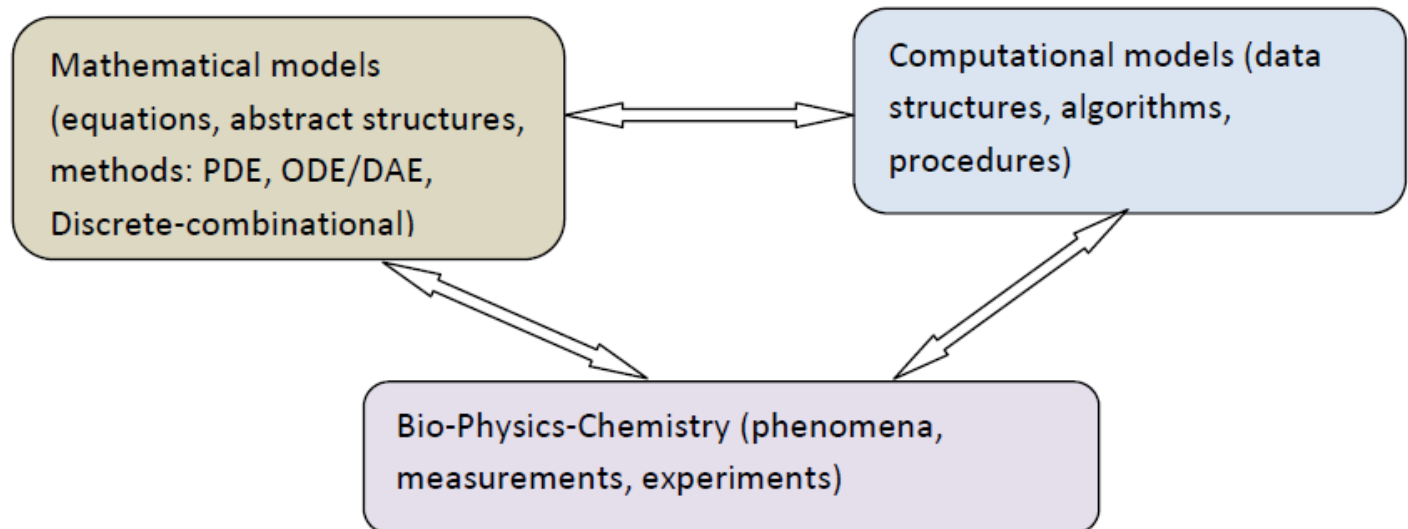
Two consecutive levels: multiscale modelling and model reduction

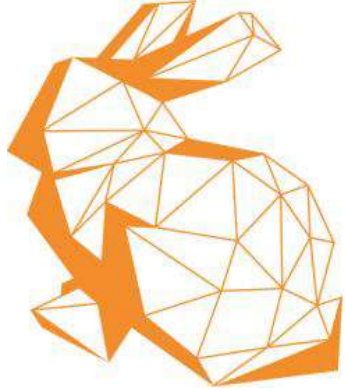




Systems Biology

- holistic as opposed to reductionist approach: system-level analysis
- hybrid: theoretical foundation consists of quantities, principles, laws and techniques from other fields such as: biology, physics, biochemistry, mathematics, control and computational sciences.





EU-MORNET

European Network for Model Reduction ★ ★ ★

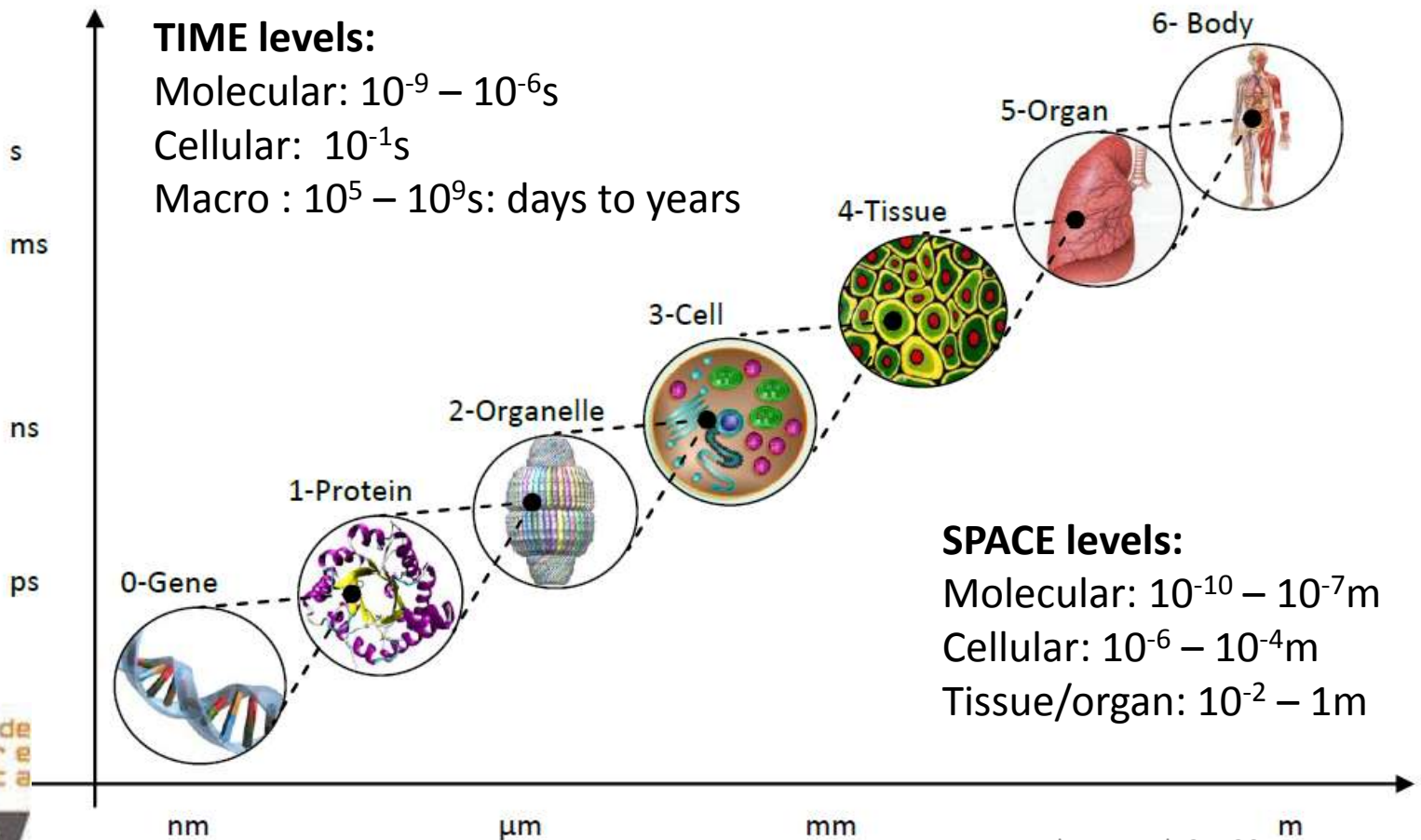


The MMM:

Multiscale

Multirate

Multiphysics





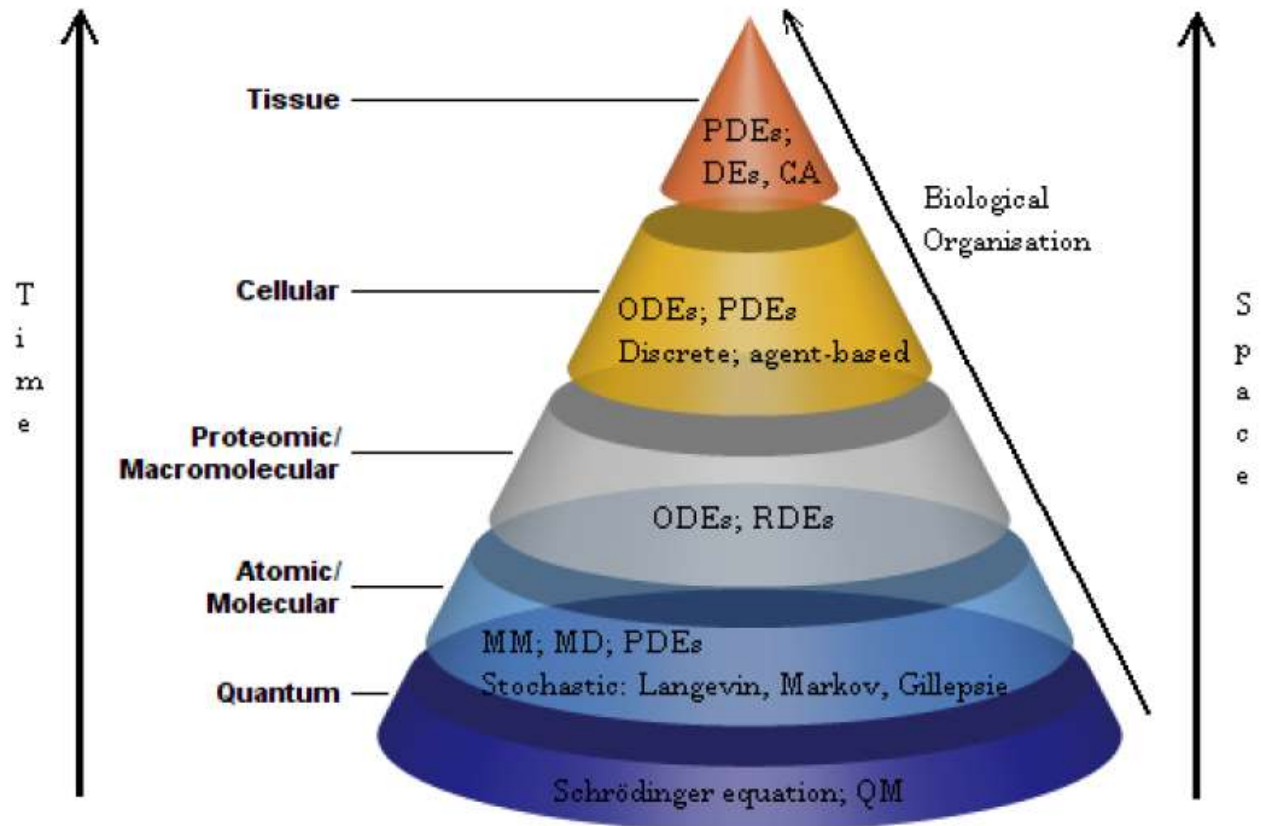
EU-MORNET

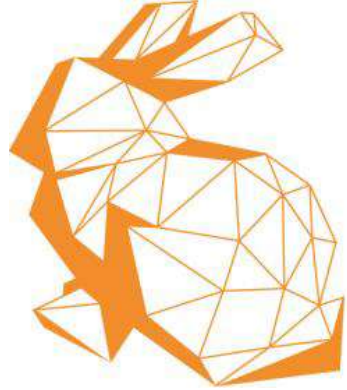
European Network for Model Reduction ★★



Abstraction levels of hierarchical biological organization:

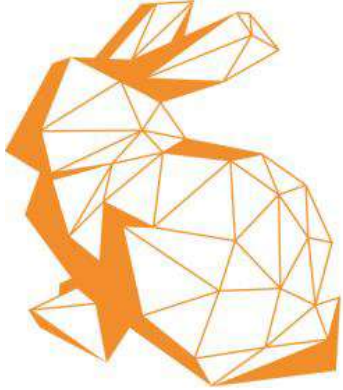
Continuous vs. discrete
Deterministic vs. stochastic



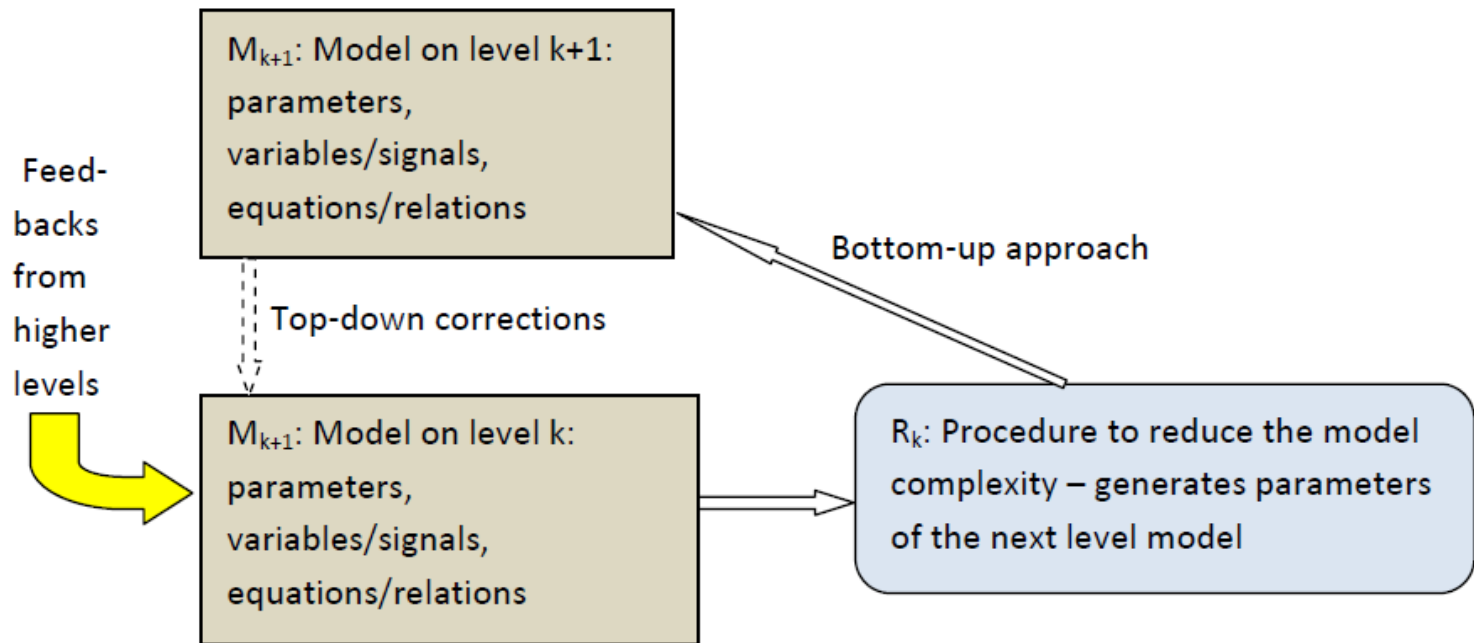


MULTI-SCALE METHODS IN MODELLING OF BIOLOGICAL SYSTEMS

QM / MM	the region of interest is represented Quantum Mechanically surrounding protein/lipid/solvent is represented at atomic scale with an empirical derived potential function
Coarse-graining	represents an idealization of various kinds mean-field theory, rule-based modelling and numerical discretization can be considered as coarse-graining methods ; also treating the cell as the smallest unit
Mean-field	can be considered a particular version of coarse-graining treats a system by assuming that the elements are controlled by a single mean field, which is created by all the elements themselves (Qu 2011) appropriate when the elements are globally coupled or when the system is well mixed
Non-linear dynamics	iterated maps manifold reduction slaving principle



Multiscale modelling and model reduction for two consecutive levels:





EU-MORNET

European Network for Model Reduction ★ ★ ★



Biological Networks

model molecular, sub-cellular and cellular processes such as: genes and protein coding, protein-protein interactions, signaling (within and between cells).

