

BioExcel

Center of Excellence for Computational Biomolecular Research

Erwin Laure

KTH Royal Institute of Technology

erwinl@pdc.kth.se

Partners



Funding



BioExcel Consortium



University of Edinburgh



KTH Royal Institute of Technology



MAX-PLANCK-GESELLSCHAFT



IRB
BARCELONA

INSTITUTE
FOR RESEARCH
IN BIOMEDICINE



Universiteit Utrecht



Ian Harrow Consulting



The University of Manchester



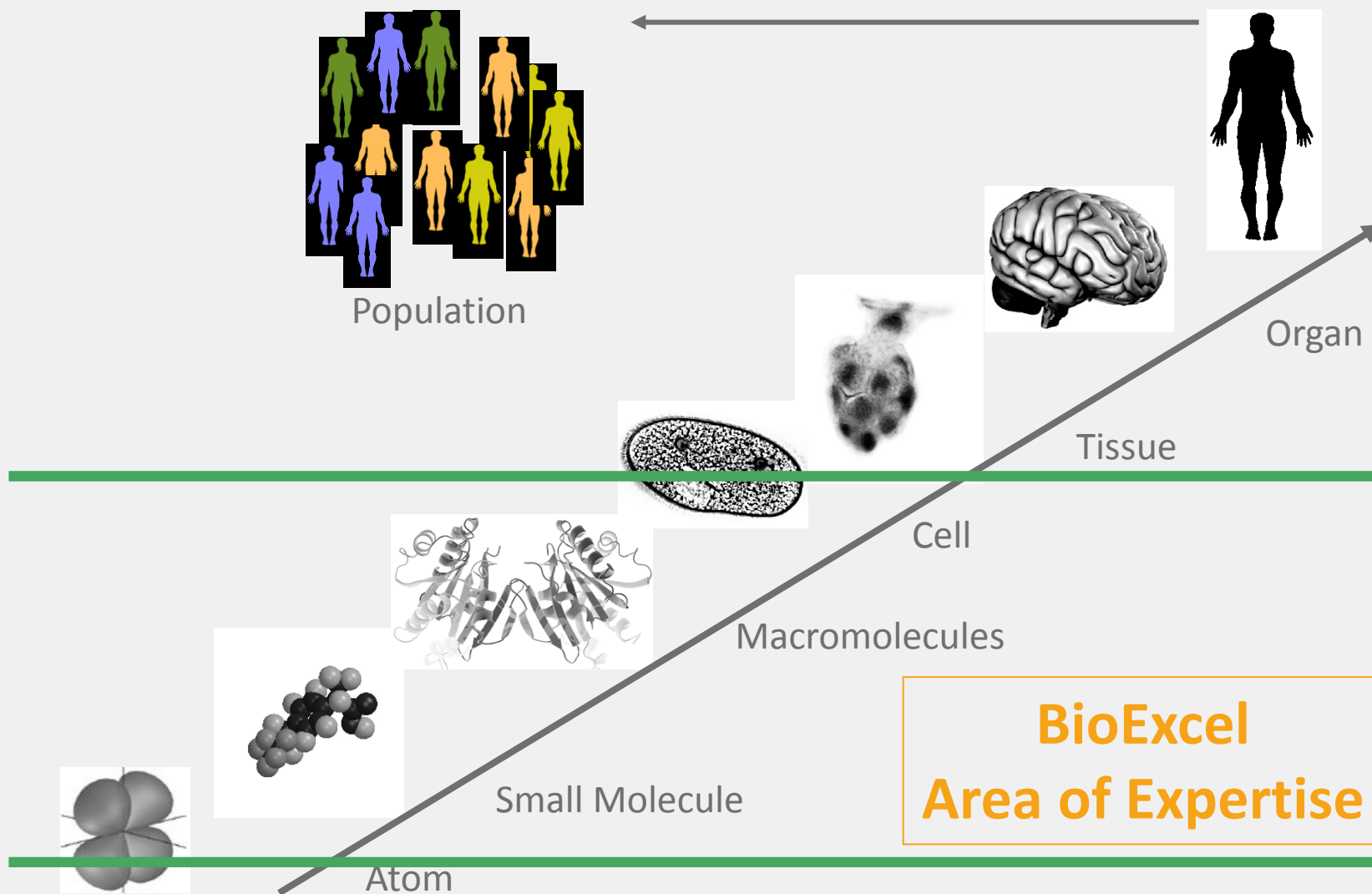
**Barcelona
Supercomputing
Center**

Centro Nacional de Supercomputación

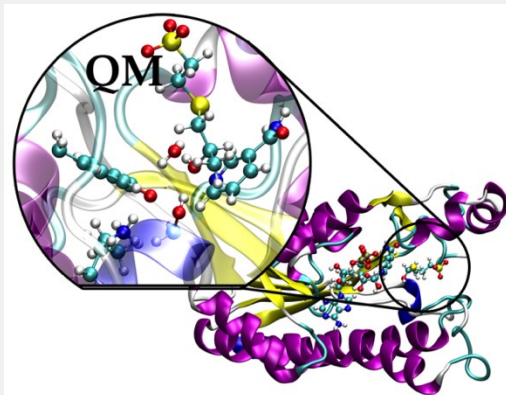
EMBL-EBI



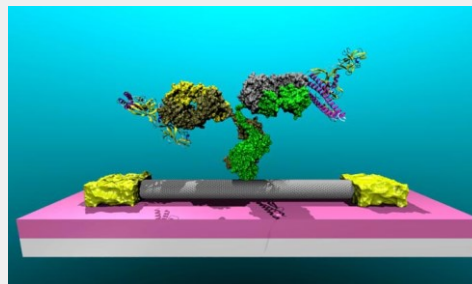
Life Science and HPC



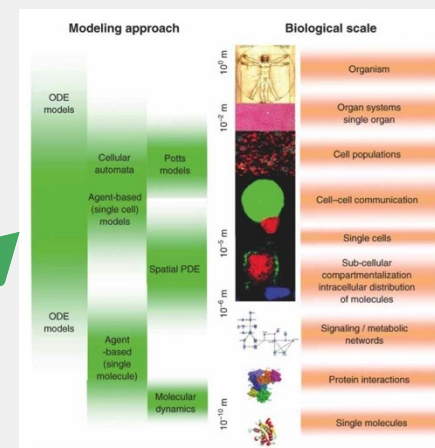
Electronic structure



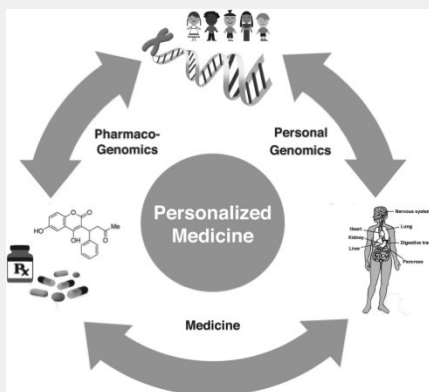
Biomarkers design



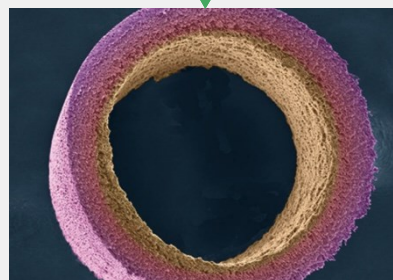
Physiology



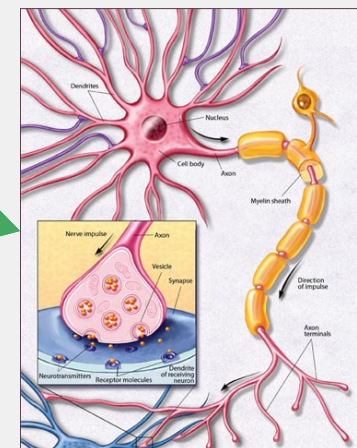
Biomolecular Modeling and Simulations



Personalized medicine



Biomaterials science and nanotechnology



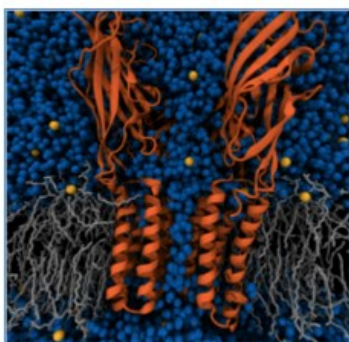
Neuroinformatics

Objectives of BioExcel

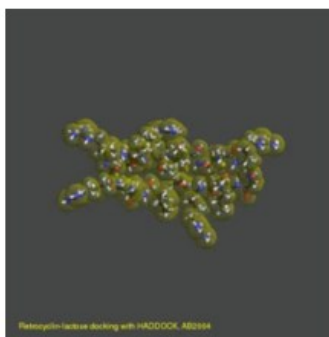
Excellence in Biomolecular Software

Improve the performance, efficiency and scalability of key codes

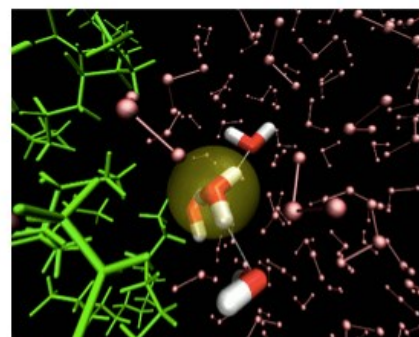
- GROMACS (Molecular Dynamics Simulations)
- HADDOCK (Integrative modeling of macro-assemblies)
- CPMD (hybrid QM/MM code for enzymatic reactions, photochemistry and electron transfer processes)



MD simulations
/GROMACS/



Docking
/HADDOCK/



QM/MM
/CPMD/

BioExcel and EsD

- Biomolecular simulations are an important usecase with special requirements
 - Need strong scaling (reasonably powerful cores)
 - Ensembles
 - All-to-all message exchange (but trying to move to neighborhood)
- Application software is essential for EsD success
 - Need more efforts on application software
 - Co-Design from the beginning!
 - Solve real scientific challenge
- CoEs play an important role in providing this software
 - But insufficient funding
 - Simply porting will be very time consuming; not to speak about optimization